

L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1992:634360 CAPLUS

DOCUMENT NUMBER: 117:234360

TITLE: Hemisynthesis of the naturally occurring tremuloidin

AUTHOR(S): Picard, Sophie; Bouyssou, Pascal; Chenault, Jacques

CORPORATE SOURCE: Lab. Chim. Bioorg. Anal. Assoc., Univ. Orleans,
Orleans, F 45067, Fr.

SOURCE: Phytochemistry (1992), 31(8), 2909-10

CODEN: PYTCAS; ISSN: 0031-9422

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:234360

AB The hemisynthesis of tremuloidin under mild conditions by
2'-O-benzoylation of salicin is described. It appears as an essential
step in synthesis of natural phenolic glycosides.

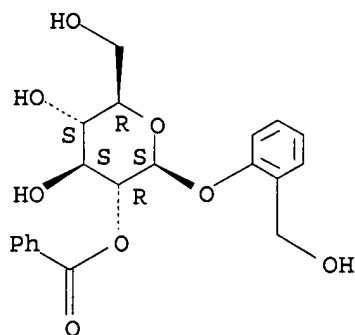
IT 529-66-8P, Tremuloidin

RL: SPN (Synthetic preparation); PREP (Preparation)
(**prepn.** of, from salicin)

RN 529-66-8 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS

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AB The hemisynthesis of tremuloidin under mild conditions by
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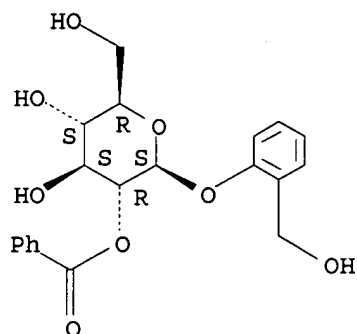
IT 529-66-8P, Tremuloidin

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, from salicin)

RN 529-66-8 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1966:29217 CAPLUS

DOCUMENT NUMBER: 64:29217

ORIGINAL REFERENCE NO.: 64:5449g-h,5450a-b

TITLE: Leaves of the family Salicaceae. V. The occurrence of glucosides in the leaves of *Populus grandidentata*

AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.

CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI

SOURCE: Tappi (1965) 48(10) 607-8
CODEN: TAPPAP; ISSN: 0039-8241

DOCUMENT TYPE: Journal

LANGUAGE: English

AB cf. CA 64, 797b. The EtOH ext. of 518 g. leaves of *P. grandidentata*, collected in June, was evapd. and yielded 133 g. sirup which was stirred with 2 l. H₂O and the granular ppt. filtered off. Extn. of the filtrate with Et₂O and evapn. of the ext. gave a mixt. of BzOH and pyrocatechol. The concd. aq. soln. was extd. with CHCl₃ and the ext. concd., giving 2.26 g. cryst. solid (I). Exhaustive extn. of the aq. soln. with EtOAc for 10, 30, 60, and 140 hrs. gave 5 g. polyphenolic material, 0.6 and 0.95 g. oligomeric material, consisting partially of salicin (II), and 1.72 g. II, resp. The aq. soln. was then dild. to 3 l. and treated with 50 g. Pb subacetate in 100 ml. H₂O, the ppt. decompd. with H₂S, and the filtered soln. evapd. in vacuo to give 0.375 g. quercitin-3-glucosiduronic acid, m. 193-5.degree. (H₂O). The filtrate of I was evapd. in vacuo, the residue dissolved in 50 ml. EtOH; 150 ml. H₂O and 7 ml. concd. H₂SO₄ in 100 ml. H₂O were added, and the mixt. was refluxed 0.5 hr. and concd. in vacuo, giving 0.263 g. salicyloylsalicin benzoate (III), m. 188-90.degree. (95% EtOH). Countercurrent distribution of I between EtOAc and H₂O gave 0.85 g. tremuloidin, m. 212-13.degree. and 0.24 g. populin (IV), m. 181-3.degree.. Extn. of 471 g. dry leaves with Et₂O gave 120 g. solid from which 1.1 g. III, and some IV and II were isolated.

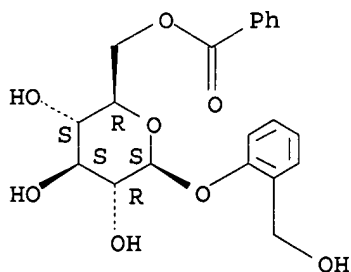
IT 99-17-2, Populin 138-52-3, Salicin 529-66-8, Tremuloidin

(in poplar leaves)

RN 99-17-2 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

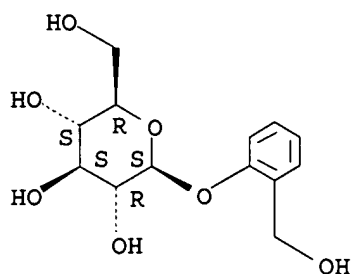
Absolute stereochemistry.



RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

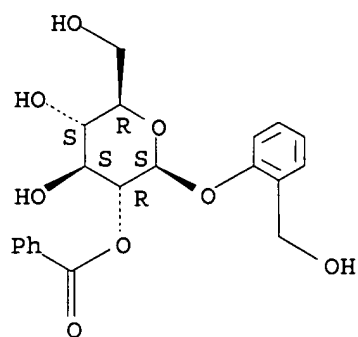
Absolute stereochemistry.



RN 529-66-8 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

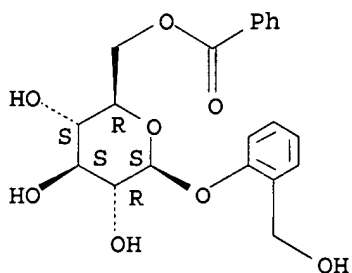


IT 99-17-2, Populin
(salicylate, in popular leaves)

RN 99-17-2 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA
INDEX NAME)

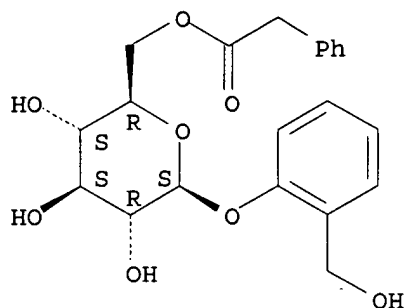
Absolute stereochemistry.



=> d scan

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI)
MF C21 H24 O8

Absolute stereochemistry.

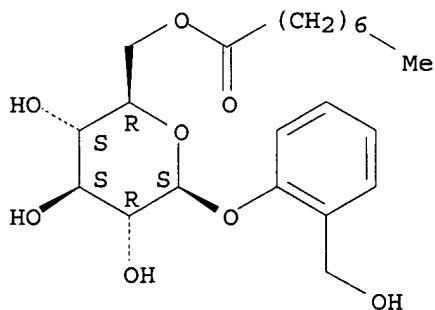


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-octanoate (9CI)
MF C21 H32 O8

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-butanoate (9CI)
MF C17 H24 O8

Absolute stereochemistry.

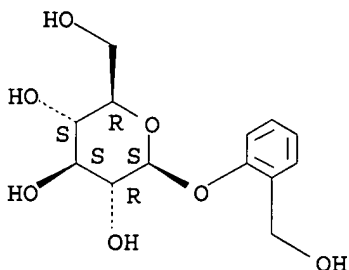
L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:727039 CAPLUS
DOCUMENT NUMBER: 137:252711
TITLE: Melanin formation promoting agents containing
salicylic acid or salicyl alcohol derivatives
INVENTOR(S): Hasegawa, Junichi; Tanaka, Kiyotaka
PATENT ASSIGNEE(S): Ichimaru Pharcos Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 30 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002275060	A2	20020925	JP 2001-75402	20010316

PRIORITY APPLN. INFO.: JP 2001-75402 20010316
OTHER SOURCE(S): MARPAT 137:252711
AB The invention relates to a melanin formation promoting agent suitable for use in a cosmetic compn. for rough skin improvement and hair growth stimulation, etc., wherein the melanin formation promoting agent contains a salicylic acid or salicyl alc. deriv. A cosmetic emulsion contg. 2-hydroxybenzoylaminoacetate 0.1 % was prepd.
IT 138-52-3
RL: COS (Cosmetic use); PAC (Pharmacological activity); BIOL (Biological study); USES (Uses)
(melanin formation promoting agents contg. salicylic acid or salicyl alc. derivs.)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1993:468105 CAPLUS
DOCUMENT NUMBER: 119:68105
TITLE: Two phenolic glucosides and an iridoid glucoside from
Alangium platanifolium var. trilobum
AUTHOR(S): Itoh, Atsuko; Tanahashi, Takao; Nagakura, Naotaka
CORPORATE SOURCE: Kobe Women's Coll. Pharm., Kobe, 658, Japan
SOURCE: Phytochemistry (1993), 33(1), 161-4
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
AB From the leaves of Alangium platanifolium var. trilobum, two new phenolic glucosides, 7-O-methylsalicin and 7-O-(2,6-dihydroxybenzoyl)salicin, and a new iridoid glucoside, 7-O-benzoylloganin, were isolated and their structures detd. by spectroscopic and chem. studies. Six known compds. isolated for the first time from this plant were

identified as salicin, quercetin-3-O-.beta.-D-glucoside, rutin, adenosine, Me caffeate and roseoside.

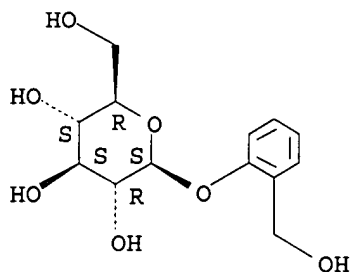
IT 138-52-3, Salicin 72021-23-9, Henryoside

RL: BIOL (Biological study)
(from Alangium platanifolium trilobium)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

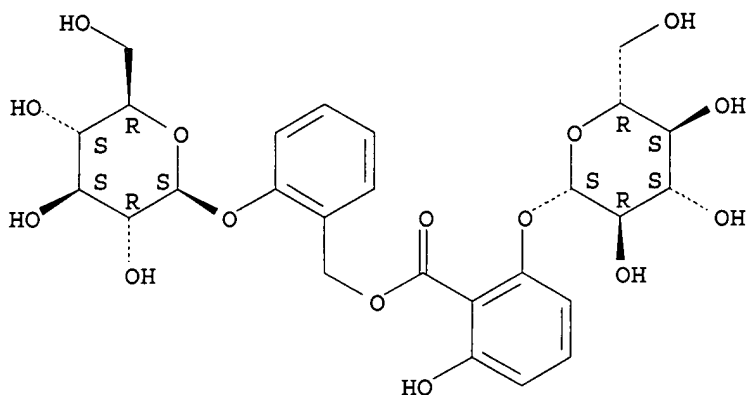
Absolute stereochemistry.



RN 72021-23-9 CAPLUS

CN .beta.-D-Glucopyranoside, 2-[[[2-(.beta.-D-glucopyranosyloxy)-6-hydroxybenzoyl]oxy]methyl]phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 148707-20-4 148707-21-5

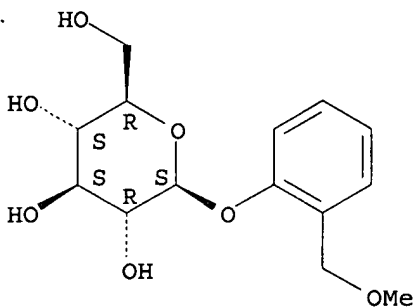
RL: BIOL (Biological study)

(isolation and structure of, from Alangium platanifolium trilobium)

RN 148707-20-4 CAPLUS

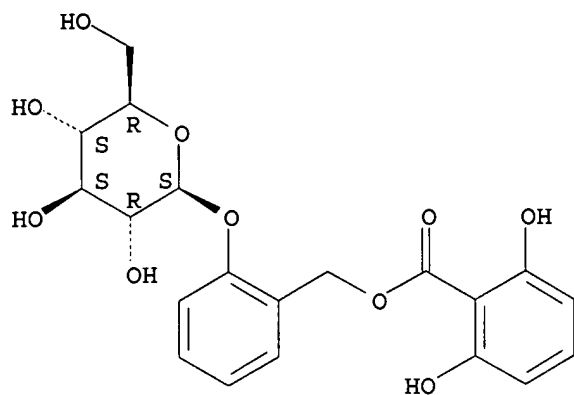
CN .beta.-D-Glucopyranoside, 2-(methoxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



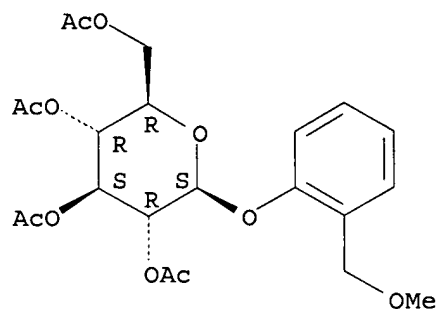
RN 148707-21-5 CAPLUS
CN .beta.-D-Glucopyranoside, 2-[[(2,6-dihydroxybenzoyl)oxy]methyl]phenyl
(9CI) (CA INDEX NAME)

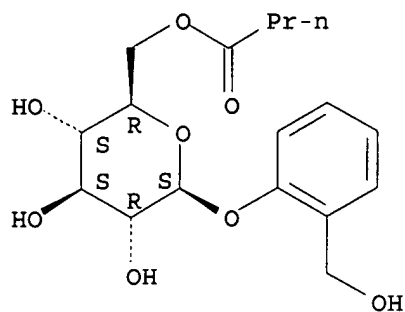
Absolute stereochemistry.



IT 148707-23-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 148707-23-7 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(methoxymethyl)phenyl, tetraacetate (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



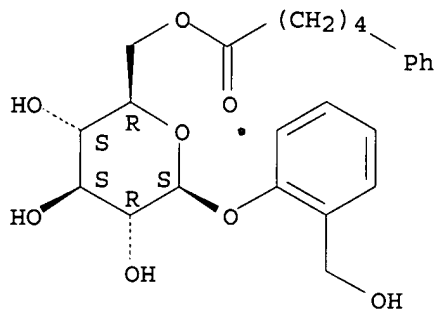


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):7

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenepentanoate
 (9CI)
 MF C24 H30 O8

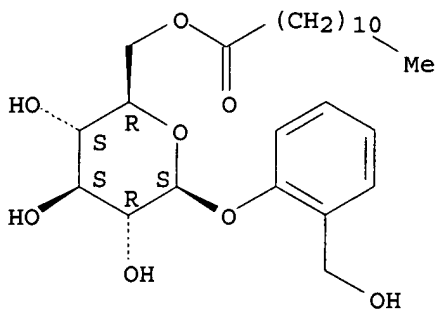
Absolute stereochemistry.

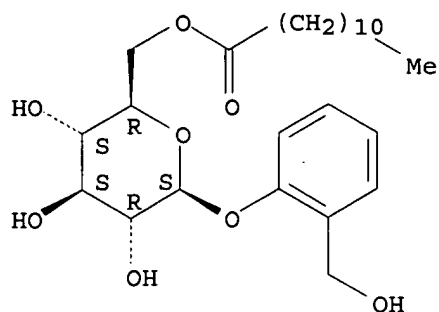


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-dodecanoate (9CI)
 MF C25 H40 O8

Absolute stereochemistry.

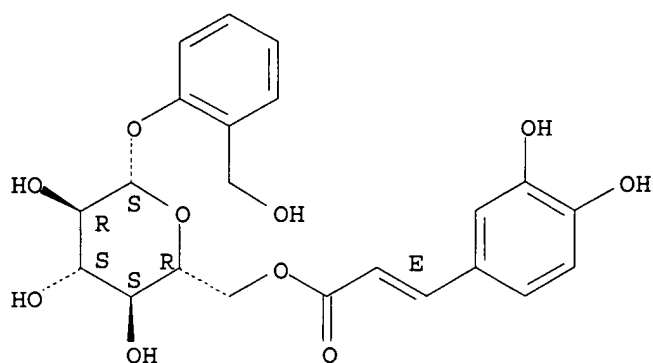




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

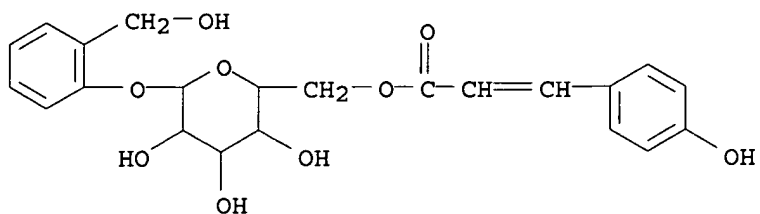
L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl 6-O-[(2E)-3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI)
 MF C22 H24 O10

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

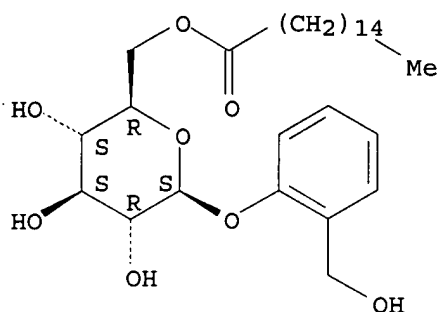
L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-[3-(4-hydroxyphenyl)-2-propenoate] (9CI)
 MF C22 H24 O9



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-hexadecanoate (9CI)
MF C29 H48 O8

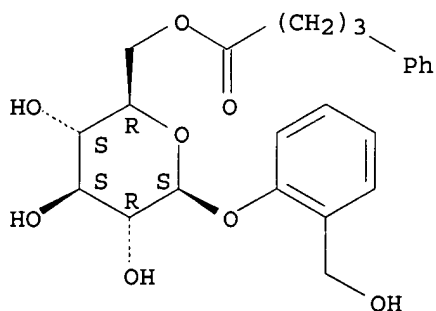
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI)
MF C23 H28 O8

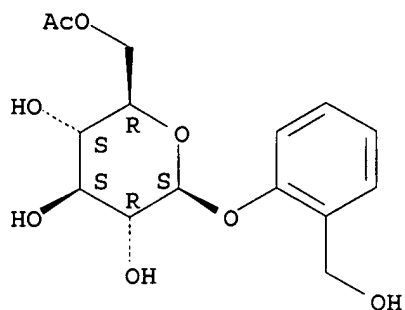
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI)
MF C15 H20 O8

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> FIL CAPLUS
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
141.42	141.63

FULL ESTIMATED COST

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FILE LAST UPDATED: 29 Nov 2002 (20021129/ED)

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=> d his

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FILE 'REGISTRY' ENTERED AT 12:59:46 ON 01 DEC 2002

L1 STRUCTURE UPLOADED
L2 0 S L1 SSS SAM
L3 10 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 13:01:55 ON 01 DEC 2002

=> s 13

L4 26 L3

=> dup rem l4

PROCESSING COMPLETED FOR L4

L5 26 DUP REM L4 (0 DUPLICATES REMOVED)

=> d l4 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 26 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:363814 CAPLUS

DOCUMENT NUMBER: 137:198580

TITLE: Preferences of six leaf beetle species among
qualitatively different leaf age classes of three
Salicaceous host species

AUTHOR(S): Ikonen, Arsi

CORPORATE SOURCE: Department of Biology, University of Joensuu, Joensuu,
FIN-80101, Finland

SOURCE: Chemoecology (2002), 12(1), 23-28

CODEN: CHMOE9; ISSN: 0937-7409

PUBLISHER: Birkhaeuser Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB As Salicaceous plants produce new leaves for a prolonged period of time, they expose a wide range of differentially aged leaves to herbivores during the growing season. In this work, it was shown that young leaves of three Salicaceous species, *Populus tremula* L., *Salix phylicifolia* L. and *S. pentandra* L., contain more nitrogen than conspecific old leaves. In *P. tremula* and *S. pentandra* young leaves also contained more low-mol. wt. secondary compds., phenolic glucosides. Leaves of *S. phylicifolia* did not contain phenolic glucosides in detectable amts. Furthermore, in *P. tremula* and *S. pentandra* young leaves contained less polymeric digestibility-reducing phenolics, condensed tannins, than old leaves. In *S. phylicifolia*, higher concns. of condensed tannins were found in young leaves. In lab. feeding trials with six leaf beetle species, young leaves of the studied plants were invariably preferred in all tested herbivore x host species combinations. In particular, it is remarkable that three leaf beetle species with known different overall relationships to phenolic glucosides equally preferred more glucoside-contg. young *S. pentandra* leaves over conspecific old ones. Four beetle species were found to prefer young leaves of *S. phylicifolia* despite the higher content of condensed tannins in young leaves. These results indicate that the general preference of leaf beetles for young leaves of Salicaceous plants probably does not primarily result from variable distribution of secondary compds. Apparently, the preference for young leaves is fundamentally due to variation in leaf nutritive traits, such as nitrogen content.

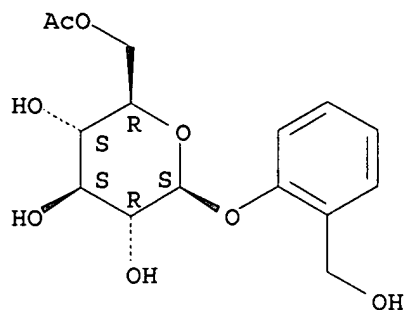
IT 19764-02-4, Fragilin

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(host preferences of leaf beetle species in relation to phenolic
glucosides and differently aged leaves of Salicaceous host species)

RN 19764-02-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:472959 CAPLUS

DOCUMENT NUMBER: 135:75834

TITLE: Enzyme-catalysed modification of substances in biological mixtures

INVENTOR(S): Otto, Ralf; Weiss, Albrecht

PATENT ASSIGNEE(S): Cognis Deutschland G.m.b.H., Germany

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046452	A1	20010628	WO 2000-EP12652	20001213
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
DE 19962204	A1	20010705	DE 1999-19962204	19991222
EP 1240349	A1	20020918	EP 2000-987394	20001213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				

PRIORITY APPLN. INFO.: DE 1999-19962204 A 19991222

WO 2000-EP12652 W 20001213

AB The invention relates to an enzyme-catalyzed modification of substances in a mixt., comprising bringing the substance in a mixt. to be modified into contact with an enzyme and a substrate. Thus, arbutin present in a com. leaf ext. of bearberry was mixed with palmitic acid in the presence of an immobilized lipase and incubated at 45 .degree.C for 24 h. The resulting palmitoyl arbutin was then extd. with chloroform or methylene chloride.

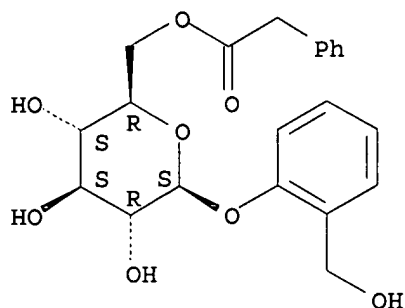
IT 270081-79-3P

RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(enzyme-catalyzed modification of compds. in biol. exts.)

RN 270081-79-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:155916 CAPLUS

DOCUMENT NUMBER: 132:344753

TITLE: Substrate specificity of lipase B from *Candida antarctica* in the synthesis of arylaliphatic glycolipids

AUTHOR(S): Otto, R. T.; Scheib, H.; Bornscheuer, U. T.; Pleiss, J.; Syltatk, C.; Schmid, R. D.

CORPORATE SOURCE: Institut für Technische Biochemie, Universität Stuttgart, Stuttgart, D-70569, Germany

SOURCE: Journal of Molecular Catalysis B: Enzymatic (2000), 8(4-6), 201-211

CODEN: JMCEF8; ISSN: 1381-1177

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Arylaliph. glycolipids are known for their pharmaceutical and medicinal properties. We found that a great variety of arylaliph. esters can be synthesized from non-activated substrates such as glucose or the naturally-occurring drug salicin using lipase B from *Candida antarctica* (CAL-B). However, esters known to display anticancer activity such as those derived from arom. carboxylic acids or unsatd. arylaliph. acids, like cinnamic acid and its derivs., could not be obtained. In this work, along with syntheses of new glycolipids, we performed computer-aided mol. modeling based on data from our recently published work to examine why some substances are accepted by CAL-B while others are not. In order to elucidate the advantages and limitations of CAL-B in the synthesis of arom. glycolipids, we investigated arylaliph. acyl donor access to the lipase binding site along with steric interactions between the glucoside aglycons and residues of the alc. binding pocket.

IT 270081-72-6P 270081-75-9P 270081-77-1P

270081-79-3P 270081-81-7P

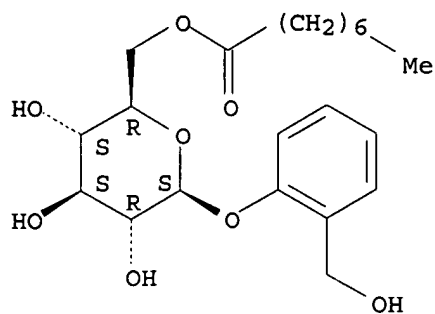
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)

(mol. modeling provides insight into substrate specificity displayed by *Candida antarctica* lipase B in synthesis of arylaliph. glycolipids)

RN 270081-72-6 CAPLUS

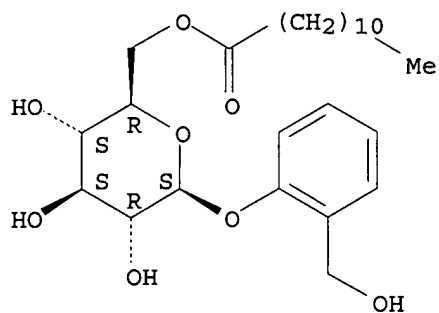
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-octanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



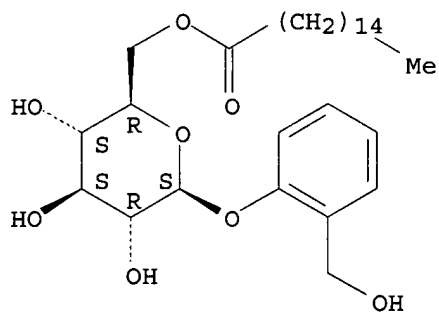
RN 270081-75-9 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-dodecanoate (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



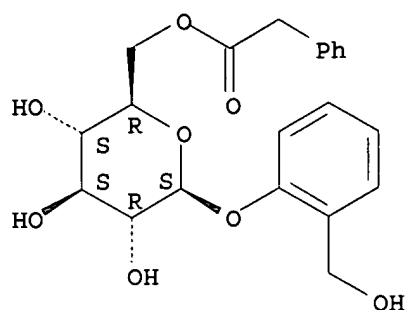
RN 270081-77-1 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-hexadecanoate (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



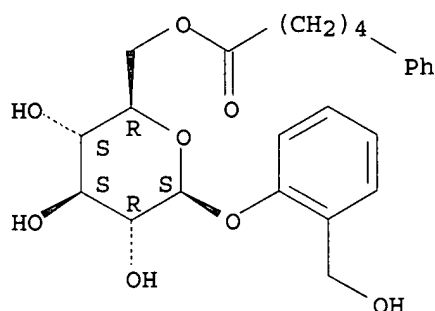
RN 270081-79-3 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 270081-81-7 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenepentanoate
 (9CI) (CA INDEX NAME)

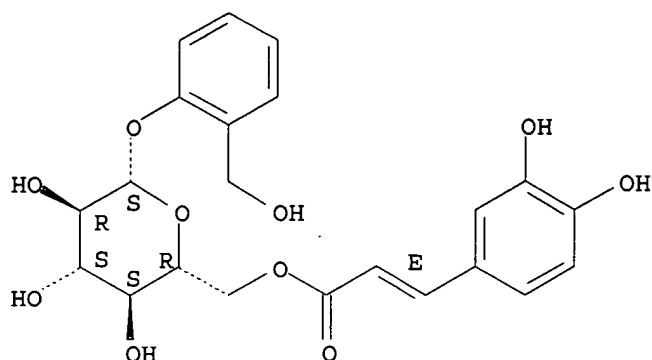
Absolute stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1999:799976 CAPLUS
 DOCUMENT NUMBER: 132:134798
 TITLE: Five Phenolic Glycosides from Alangium chinense
 AUTHOR(S): Itoh, Atsuko; Tanahashi, Takao; Ikejima, Sanae; Inoue, Miho; Nagakura, Naotaka; Inoue, Kenichiro; Kuwajima, Hiroshi; Wu, Hua-Xin
 CORPORATE SOURCE: Kobe Pharmaceutical University, Higashinada-ku Kobe, 658-8558, Japan
 SOURCE: Journal of Natural Products (2000), 63(1), 95-98
 CODEN: JNPRDF; ISSN: 0163-3864
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB From the dried leaves of Alangium chinense, five novel phenolic glycosides, 6'-O-galloylsalicin, 4',6'-di-O-galloylsalicin, 4',6'-O-(S)-hexahydroxydiphenoylsalicin, 4',6'-O-(R)-hexahydroxydiphenoylsalicin, and pyrocatechol 1-O-.beta.-D-xylopyranosyl(1.fwdarw.6)-.beta.-D-glucopyranoside were isolated. The structures of these new compds. were detd. by spectroscopic methods.
 IT 193280-04-5P, 6'-O-trans-Caffeoylsalicin
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (phenolic glycosides from Alangium chinense)
 RN 193280-04-5 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl 6-O-[(2E)-3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1999:393069 CAPLUS
 DOCUMENT NUMBER: 131:43666
 TITLE: Method for selective esterification of polyols
 INVENTOR(S): Otto, Ralf; Syldatk, Christoph; Cao, Linqiu;
 Bornscheuer, Uwe; Schmid, Rolf D.
 PATENT ASSIGNEE(S): Henkel K.-G.a.A., Germany
 SOURCE: Ger. Offen., 8 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19753789	A1	19990617	DE 1997-19753789	19971204

OTHER SOURCE(S): CASREACT 131:43666; MARPAT 131:43666

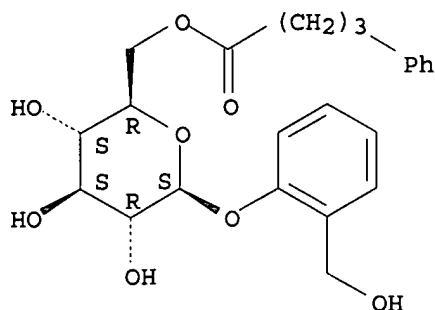
AB The prodn., from the corresponding polyol and carboxylic acid contg. an arom. ring, of polyols esterified on the primary -OH group is improved in selectivity and yield without introducing and removing protecting groups. This is characterized in that the polyol and carboxylic acid, in the presence of a small amt. of org. solvent that dissolves neither completely, react with each other under catalysis by a lipase or an esterase. The products have emulsifying activity with potential pharmaceutical use.

IT **218966-96-2P**
 RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (selective esterification of polyols)

RN 218966-96-2 CAPLUS

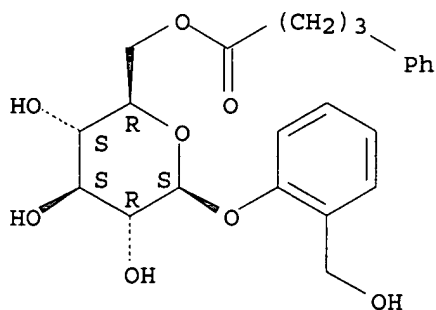
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI) (CA INDEX NAME)

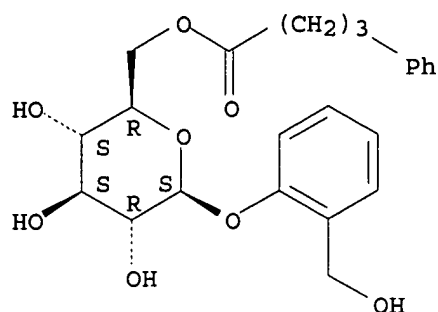
Absolute stereochemistry.



L4 ANSWER 6 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1998:708306 CAPLUS
 DOCUMENT NUMBER: 130:80398
 TITLE: Lipase-catalyzed synthesis of arylaliphatic esters of .beta.-D(+)-glucose, n-alkyl- and arylglucosides and characterization of their surfactant properties
 AUTHOR(S): Otto, Ralf T.; Bornscheuer, Uwe T.; Syltschik, Christoph; Schmid, Rolf D.
 CORPORATE SOURCE: Institut für Bioverfahrenstechnik, Universität Stuttgart, Stuttgart, D-70569, Germany
 SOURCE: Journal of Biotechnology (1998), 64(2,3), 231-237
 CODEN: JBITD4; ISSN: 0168-1656
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB .beta.-D(+)-Glucose, n-alkyl-.beta.-D(+)-glucosides, salicin and 1-phenylglucoside were regioselectively acylated at the primary hydroxy group of the sugar moiety with a variety of non-activated arylaliph. carboxylic acids using lipase B from *Candida antarctica* in a mainly solid phase in the presence of a small amt. of t-butanol in yields up to 71%. The arylaliph. glucose esters were highly water sol. (15 to 100 g l⁻¹) and showed surface activity. Crit. micellar concns. between 2 and 95 mM and minimal surface tensions around 35-45 mN m⁻¹ were detd. The hydrophilic-lipophilic balance values of arylaliph. esters from .beta.-D(+)-glucose indicate a use in oil-in-water emulsions or detergents, whereas the n-alkyl- and arylglycosides can be employed as wetting agents or water-in-oil emulsifiers.
 IT **218966-96-2P**
 RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
 (lipase-catalyzed synthesis of arylaliph. esters of .beta.-D(+)-glucose, n-alkyl- and arylglucosides and characterization of their surfactant properties)
 RN 218966-96-2 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.





REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:505793 CAPLUS

DOCUMENT NUMBER: 127:147088

TITLE: Two new phenolic glycosides from *Alangium chinense*

AUTHOR(S): Itoh, Atsuko; Tanahashi, Takao; Nagakura, Naotaka

CORPORATE SOURCE: Kobe Pharmaceutical University, Kobe, 658, Japan

SOURCE: Natural Medicines (Tokyo) (1997), 51(2), 173-175

CODEN: NMEDEO; ISSN: 1340-3443

PUBLISHER: Japanese Society of Pharmacognosy

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB From the leaves of *Alangium chinense* (LOUR.) HARMS, two novel glycosides, 6'-O-.beta.-D-xylopyranosylsalicin and 6'-O-trans-caffeoylsalicin, were isolated and their structures detd. on the basis of spectroscopic data.

IT 193280-04-5P, 6'-O-trans-Caffeoylsalicin

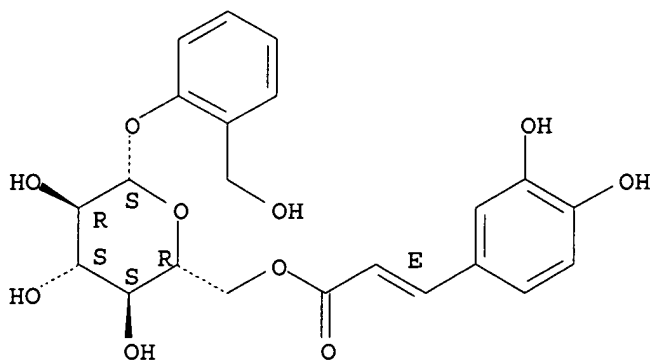
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(phenolic glycosides from *Alangium chinense*)

RN 193280-04-5 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl 6-O-[(2E)-3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L4 ANSWER 8 OF 26 CAPLUS COPYRIGHT 2002 ACS

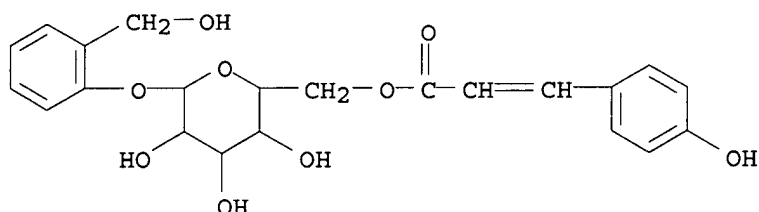
ACCESSION NUMBER: 1996:668128 CAPLUS

DOCUMENT NUMBER: 125:323005

TITLE: Chemical studies on antituberculosis compounds from *Salix capitata*

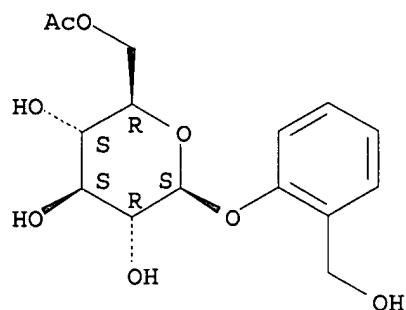
AUTHOR(S): Keapigu, M. C.; Wang, Mingshi

CORPORATE SOURCE: Dep. of Phytochemistry, China pharmaceutical Univ.,
Nanjing, 210009, Peop. Rep. China
SOURCE: Zhongguo Yaoke Daxue Xuebao (1996), 27(5), 271-273
CODEN: ZHYXE9; ISSN: 1000-5048
PUBLISHER: Zhongguo Yaoke Daxue
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Ten constituents were isolated from the tender leaves of *S. capitate*, and identified as .beta.-sitosterol, stigmasterol, p-hydroxystyrene, cinnamic acid, salicyl alc., pyrocatechol, protocatechuic acid, daucosterol, salicin, and trichocarposide. P-hydroxystyrene was effective in inhibiting human mycobacterium tuberculosis. The structure of trichocarposide was cor. according to the exptl. data.
IT 17063-94-4, Trichocarposide
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(antituberculosis compds. from *Salix capitata*)
RN 17063-94-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-[3-(4-hydroxyphenyl)-2-propenoate] (9CI) (CA INDEX NAME)



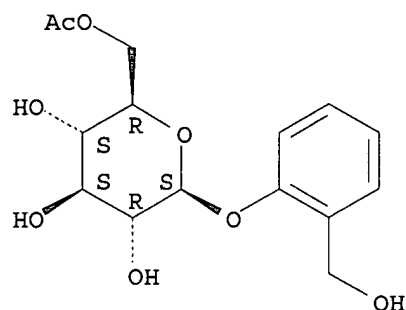
L4 ANSWER 9 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:652067 CAPLUS
DOCUMENT NUMBER: 115:252067
TITLE: Extractive substances of bast, ligneous tissue, and fiber of flax straw
AUTHOR(S): Karpunin, I. I.; Murashkevich, T. V.
CORPORATE SOURCE: Beloruss NII Lenu, USSR
SOURCE: Vestsi Akademii Navuk BSSR, Seryya Khimichnykh Navuk (1991), (2), 59-64
CODEN: VBSKAK; ISSN: 0002-3590
DOCUMENT TYPE: Journal
LANGUAGE: Belorussian
AB Glycosides and flavonols were lower in flax fiber than in the ligneous tissue and bast. Anthocyanins were high in the bast and low in the ligneous tissue and fiber. A bast constituent, 5,7,4-trihydroxyflavanone-5-(6-o-p-coumaroyl)glucopyranoside, known formerly from *Salix* bark, was identified for the first time in flax.
IT 19764-02-4, Fragilin
RL: BIOL (Biological study)
(of flax straw fractions)
RN 19764-02-4 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 10 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1990:18845 CAPLUS
 DOCUMENT NUMBER: 112:18845
 TITLE: Phenolic constituents of Salix: a chemotaxonomic survey of further Finnish species
 AUTHOR(S): Julkunen-Tiitto, R.
 CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, 80101, Finland
 SOURCE: Phytochemistry (1989), 28(8), 2115-25
 CODEN: PYTCAS; ISSN: 0031-9422
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Various parts of some 30 Salix (willow) species were screened for 14 simple phenolic glucosides and salicyl alc. Species-specific qual. and quant. variation of phenolic glucosides in willow species was considerable and dependent on the part of the plant examd. Generally, there was greater diversity in glucoside compn. and a higher total amt. of glucosides in the twigs than in the leaves and buds. The traditional classification turned out to be inconsistent with a classification based on phenolic glucosides only. However, simple phenolic glucosides can be used for the recognition of exomorphol. similar species and hybrid forms. Salicyl alc. was not detected in any of the willow exts.
 IT 19764-02-4, Fragilin
 RL: BIOL (Biological study)
 (of Salix species, chemotaxonomy in relation to)
 RN 19764-02-4 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

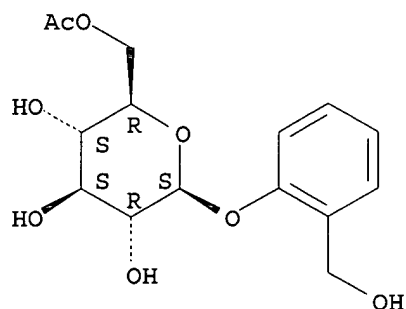
Absolute stereochemistry.



L4 ANSWER 11 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1989:406459 CAPLUS
 DOCUMENT NUMBER: 111:6459
 TITLE: Carbon-nutrient balance hypothesis in within-species phytochemical variation of Salix lasiolepis
 AUTHOR(S): Price, Peter W.; Waring, Gwendolyn L.;

Julkunen-Tiitto, Riitta; Tahvanainen, Jorma; Mooney, Harold A.; Craig, Timothy P.
 CORPORATE SOURCE: Dep. Biol. Sci., North. Arizona Univ., Flagstaff, AZ, 86011, USA
 SOURCE: Journal of Chemical Ecology (1989), 15(4), 1117-31
 CODEN: JCECD8; ISSN: 0098-0331
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Predictions of the carbon-nutrient balance hypothesis were tested using a study of within-species phytochem. variation of the arroyo willow, *S. lasiolepis*. The prediction that a balance between nutrients (total protein) and carbon-based secondary metabolites (total phenols) should exist was supported using water treatment and fertilizer expts. and wild willow clones. Leaf nitrogen content and net photosynthetic rates of plants potted in soil in which parental plants grew was low, indicating that wild plants exist under relatively low nutrient status-high carbon balance conditions. The hypothesis also correctly predicted pos. relationships between shoot length and phenols in glasshouse plants, wild plants, and plants in the water treatment expt. and neg. relationships between shoot length and phenols in the fertilizer treatment expt. Total phenolic glycosides, fragilin, picetin, salicortin, tremulacin, and tremuloidin all correlated pos. with shoot length in glasshouse plants on a carbon-biased balance, and male willows had generally lower levels of phenolic glycosides than females. Salicortin and tremulacin showed the strongest pos. relationships with shoot length.
 IT 19764-02-4
 RL: BIOL (Biological study)
 (of *Salix lasiolepis*, shoot length in relation to)
 RN 19764-02-4 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

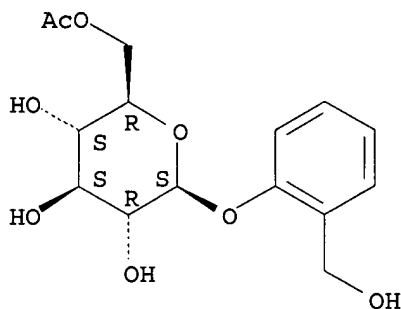


L4 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1989:403512 CAPLUS
 DOCUMENT NUMBER: 111:3512
 TITLE: The effect of the sample preparation method of extractable phenolics of Salicaceae species
 AUTHOR(S): Julkunen-Tiitto, R.; Tahvanainen, J.
 CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, SF-80101, Finland
 SOURCE: Planta Medica (1989), 55(1), 55-8
 CODEN: PLMEAA; ISSN: 0032-0943
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The effect of different tissue prehandling methods on the phenolic content of willow bark, leaves, and twigs was studied. The phenolics were extd. at room temp., purified, and analyzed by high-resoln. capillary gas chromatog. Neither oven drying at a low temp. nor room drying of fresh leaves and oven drying of bark produced any qual. changes in the glucoside

compn. and only a minor binding effect was seen on the amts. of each glucoside. On the other hand, oven drying of the intact long twigs and room drying of the bark are prehandling methods to avoid. Freeze drying or immediate anal. of frozen leaves lowered the total amt. of glucosides and caused considerable qual. changes to the glucoside compn. Acetone (80%) was a slightly more effective and gentle extn. solvent for all glucosides compared with methanol.

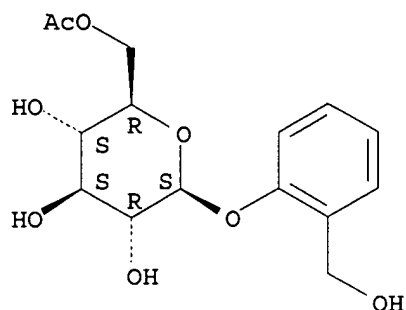
IT 19764-02-4, Fragilin
 RL: ANT (Analyte); ANST (Analytical study)
 (detn. of, in willow by gas chromatog., sample prepn. method effect on)
 RN 19764-02-4 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 13 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1988:489072 CAPLUS
 DOCUMENT NUMBER: 109:89072
 TITLE: Comparative high-performance liquid and gas-liquid chromatographic determination of phenolic glucosides in Salicaceae species
 AUTHOR(S): Meier, B.; Julkunen-Tiitto, R.; Tahvanainen, J.; Sticher, O.
 CORPORATE SOURCE: Dep. Pharm., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.
 SOURCE: Journal of Chromatography (1988), 442, 175-86
 CODEN: JOCRAM; ISSN: 0021-9673
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The phenolic glucosides of 7 willow species with different glucoside patterns were extd., purified, and analyzed by GC and HPLC. Two sample prepn. methods were used. It was shown that the HPLC and GC methods give comparable qual. and quant. results for the phenolic glucoside contents of the tested willows. Consequently, both methods can be used for species-specific screening of the glucoside patterns of Salicaceae species.
 IT 19764-02-4, Fragilin
 RL: ANT (Analyte); ANST (Analytical study)
 (detn. of, in willow species by GC and HPLC)
 RN 19764-02-4 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 14 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:52346 CAPLUS

DOCUMENT NUMBER: 108:52346

TITLE: Protease-catalyzed regioselective esterification of sugars and related compounds in anhydrous dimethylformamide

AUTHOR(S): Riva, Sergio; Chopineau, Joel; Kieboom, A. P. G.; Klibanov, Alexander M.

CORPORATE SOURCE: Dep. Appl. Biol. Sci., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA

SOURCE: Journal of the American Chemical Society (1988), 110(2), 584-9

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

AB By taking advantage of the unique dissolving potency of DMF and the broad substrate specificity of subtilisin, a no. of carbohydrates and other sugar-contg. compds. were regioselectively acylated via enzymic transesterification. Monobutyryl esters of the disaccharides maltose, cellobiose, lactose, and sucrose were prepd. readily on a gram scale. The presence of a bulky aglycon moiety does not substantially reduce the catalytic efficiency of subtilisin in DMF, thus permitting preparative enzymic esterification of natural compds. such as riboflavin, salicin, and the nucleosides adenosine and uridine. The reactivity of subtilisin only modestly drops upon an increase in the size of the carbohydrate substrate from maltose to maltoheptose. In addn. to the butyryl group, various N-acetylamino acid residues were enzymically introduced into sugars. Both highly purified and crude preps. of subtilisin were used successfully as practical catalysts of transesterifications in dry DMF.

IT 111933-84-7P

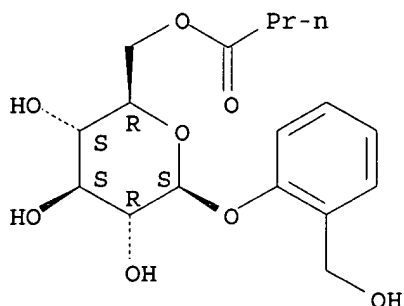
RL: PREP (Preparation)

(prepn. of, by esterification of subtilisin in anhyd. DMF)

RN 111933-84-7 CAPLUS

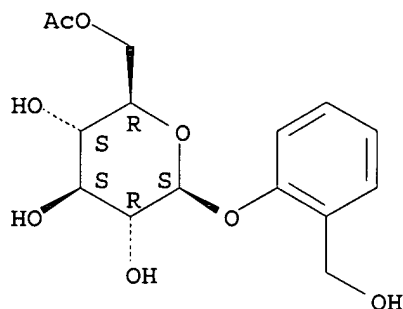
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-butanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1988:34778 CAPLUS
 DOCUMENT NUMBER: 108:34778
 TITLE: Phenolics in the leaves and twigs of *Salix pentandra* L. (Salicaceae)
 AUTHOR(S): Julkunen-Tiitto, R.
 CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, Finland
 SOURCE: Bulletin de Liaison - Groupe Polyphenols (1986), 13, 583-5
 CODEN: BLPLAS; ISSN: 0242-8466
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The seasonal variations of phenolic glucosides (salicin, fragilin, picein, and salicortin) in leaves and twigs of *S. pentandra* are reported. The concn. of total phenolics in the leaves and current growth twigs continuously increased during the growing season reaching its highest value in mid-Sept.; before winter dormancy and leaf abscission a .apprx.50% drop in total phenolics occurred.
 IT 19764-02-4, Fragilin glycoside
 RL: PROC (Process)
 (in leaves and twigs of *Salix pentandra*, seasonal variation of)
 RN 19764-02-4 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



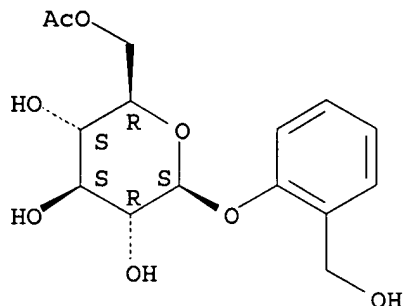
L4 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1985:218406 CAPLUS
 DOCUMENT NUMBER: 102:218406
 TITLE: Chemotaxonomical screening of phenolic glycosides in northern willow twigs by capillary gas chromatography
 AUTHOR(S): Julkunen-Tiitto, R.
 CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, SF-80101/10, Finland
 SOURCE: Journal of Chromatography (1985), 324(1), 129-39
 CODEN: JOCRAM; ISSN: 0021-9673
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The phenolic glycosides in the twig tissues of willows and common aspen (Salicaceae) were extd., purified, and chromatographed using a SE-52 column. The glycosides screened were salicin, fragilin, picein, salidroside, vimalin, triandrin, tremuloidin, populin, salicortin, and grandidentatin. Each species exhibited a typical glycoside compn., which could change during the plant's life span. The glycosidic spectra may be used with certain reservations for the identification of unknown *Salix* and *Populus* species.
 IT 19764-02-4
 RL: BIOL (Biological study)

(of aspen and willow species, in twigs, taxonomy in relation to)

RN 19764-02-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 17 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1973:156653 CAPLUS

DOCUMENT NUMBER: 78:156653

TITLE: Phenolic glycosides of Salix pentandroides roots

AUTHOR(S): Kompantsev, V. A.; Shinkarenko, A. L.

CORPORATE SOURCE: Pyatigorsk. Farm. Inst., Pyatigorsk, USSR

SOURCE: Khim. Prir. Soedin. (1973), 9(1), 126

CODEN: KPSUAR

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The fresh bark of 2-5-years-old *S. pentandroides* collected in June was extd. with EtOH-MeOH (1:1). The ext. was evapd. in vacuo, dild. with H₂O, purified by extn. with CHCl₃, pptd. with Pb subacetate, and the filtrate extd. with EtOAc. The cryst. glycoside obtained yielded on hydrolysis HOAc and salicin; it was identified as fragilin. After the removal of fragilin the EtOAc ext. was analyzed on a cellulose column. Fractional elution with BuOH-toluene-H₂O (4:6:8) yielded (42-56th 50-ml fraction) salicin.

IT 19764-02-4

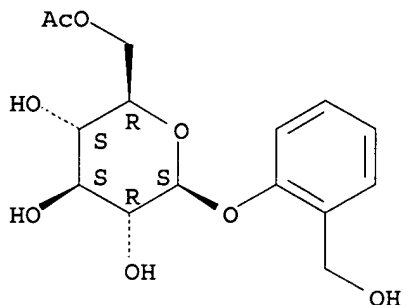
RL: BOC (Biological occurrence); BIOL (Biological study); OCCU
(Occurrence)

(of *Salix pentandroides*)

RN 19764-02-4 CAPLUS

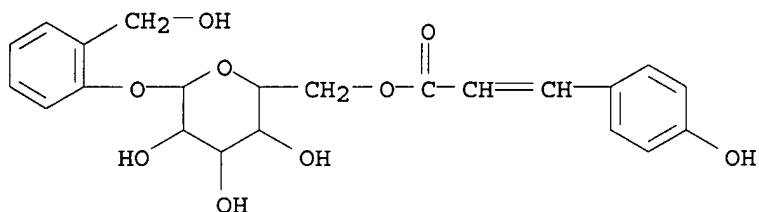
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



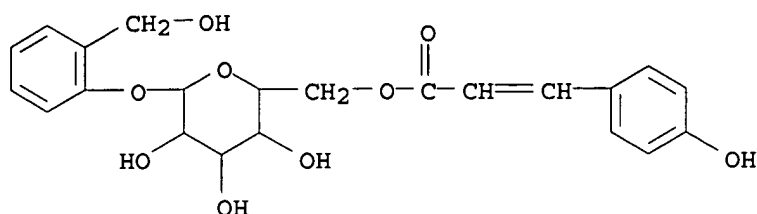
L4 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1971:61582 CAPLUS
 DOCUMENT NUMBER: 74:61582
 TITLE: Barks of the family Salicaceae. XXVI. Hot water extractives of the bark and leaves of *Populus deltoides*
 AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
 CORPORATE SOURCE: Inst. Paper Chem., Appleton, Wis., USA
 SOURCE: Can. J. Chem. (1971), 49(1), 49-55
 CODEN: CJCHAG
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The hot water extractives of the fresh smooth green bark and the fresh leaves of a *P. deltoides* tree cut in June and homogenized in EtOH were extd. fractionally with EtOAc, and the individual EtOAc exts. were fractionated by elution chromatog. with water, 20% EtOH, and 50% EtOH on polyamide columns. Important components found in the bark were salicortin, salicin, salicyl alc., pyrocatechol, .omega.-salicyloylsalicin, grandidentatin, grandidentoside, populoside, trichocarposide, and 6-methylidihydroquercetin. Important components found in the leaves were salicortin, salicin, salicyl alc., pyrocatechol, 1-O-p-coumaroyl-.beta.-D-glucoside, populoside, .omega.-salicyloylsalicin, chrysin-7-glucoside, and a new glucoside, deltoidin, which has been identified as 2-O-salicyloylsalicin.
 IT **17063-94-4**
 RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)
 (of *Populus deltoides*)
 RN 17063-94-4 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-[3-(4-hydroxyphenyl)-2-propenoate] (9CI) (CA INDEX NAME)



L4 ANSWER 19 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1970:97305 CAPLUS
 DOCUMENT NUMBER: 72:97305
 TITLE: Barks of the family Salicaceae. XXIII. Investigation of the hot-water extractives of *Populus balsamifera* bark
 AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
 CORPORATE SOURCE: Inst. of Paper Chem., Appleton, Wis., USA
 SOURCE: Phytochemistry (1969), 8(12), 2393-6
 CODEN: PYTCAS
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A no. of components were found in *P. balsamifera* bark which were not previously recorded from this important pulpwood species. These are salicortin, trichocarposide, populoside, salicyloylsalicin, and dihydromyricetin. A new procedure for chromatog. on polyamide columns gave a greater recovery than previously obtained.
 IT **17063-94-4**
 RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)
 (of *Populus balsamifera*)

RN 17063-94-4 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-[3-(4-hydroxyphenyl)-2-propenoate] (9CI) (CA INDEX NAME)



L4 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1970:18977 CAPLUS

DOCUMENT NUMBER: 72:18977

TITLE: Separation of phenolic glucosides by gel filtration

AUTHOR(S): Repas, A.; Nikolin, B.; Dursun, K.

CORPORATE SOURCE: Univ. Sarajevo, Sarajevo, Yugoslavia

SOURCE: J. Chromatogr. (1969), 44(1), 184-7

CODEN: JOCRAM

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The method of gel filtration was applied to the sepn. of more complex mixts. of naturally occurring phenolic glucosides. The freshly obtained bark of various Salicaceae species was extd. with 96% EtOH and the ext. was treated with an excess of basic lead acetat e. The mixt. was filtered, and Pb removed from the clear filtrate by treatment with H₂S. The phenolic glucosides (10-15 mg sample in 2-3 ml eluent) were sepd. on Sephadex G-25 or Sephadex LH-20 by using water, H₂O-EtOH (9:1), H₂O-MeOH (9:1), or 96% EtOH as eluents and H₂SO₄ as the colorim etric reagent. The absorbance of the colored salicin-H₂SO₄ complex was max. at 510 m.mu.. The fractionated glucosides were identified by thin-layer chromatog. on silica gel in a CHCl₃-MeOH (4:1) system. Salicin, populin, tremuloidin, salireposide, and grandidentatin were best sepd. on Sephadex G-25 with H₂O-EtOH (9:1) or H₂O-MeOH (9:1). In all cases, fragilin and triandrin were eluted simultaneously with salicin.

IT 19764-02-4

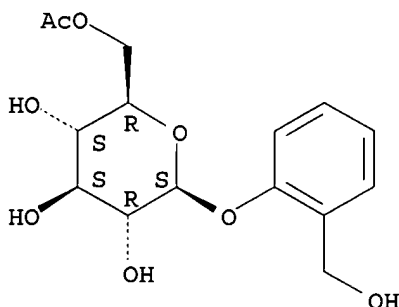
RL: PROC (Process)

(sepn. of, by gel filtration)

RN 19764-02-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

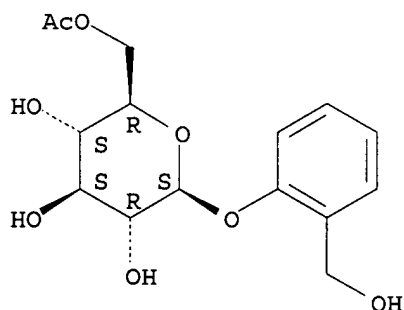
Absolute stereochemistry.



L4 ANSWER 21 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1968:457517 CAPLUS
 DOCUMENT NUMBER: 69:57517
 TITLE: Phytochemistry of Salix species. I. A gas-liquid chromatographic procedure for the separation of phenolic glycosides
 AUTHOR(S): Bolan, M.; Steele, J. W.
 CORPORATE SOURCE: Sch. Pharm., Univ. Manitoba, Winnipeg, Manitoba, Can.
 SOURCE: J. Chromatogr. (1968), 36(1), 22-30
 CODEN: JOCRAM
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Ten phenolic glycosides commonly found in Salix species were sepd. and identified by gas-liq. chromatog. of the trimethylsilyl ether derivs. The derivs. were prepd. by dissolving 0.01-0.05 mg. of pure glycoside or 0.1-0.3 mg. of natural or artificial mixts. in 50 .mu.l. Tri-Sil, shaking, and allowing the mixt. to stand 15 min. at room temp. before chromatog. He carrier gas, a flame ionization detector, and acid-washed, Me2SiCl2-treated column supports were used. All 10 glycosides were sepd. on a 0.5% cyclohexanedimethanol succinate/Chromosorb G column, although the peaks for salidroside (I) and fragilin (II) had overlapping bases. The glycoside and retention time relative to trimethylsilyl arbutin are, resp.: salicin (III), 0.64; I, 1.65; II, 1.75; picein (IV), 2.41; triandrin, 2.70; vimalin, 2.86; populin, 3.30; tremuloidin, 3.23; salireposide, 3.54; grandidentatin, 4.21. A 0.3% OV-1/Chromosorb G column completely resolved I. II was sepd. from all other components on a 0.2% OV-17/Chromosorb G column. A 1.5% diethylene glycol succinate (DEGS)/Chromosorb W column tended to cause some tailing of the peaks but was useful for obtaining addnl. evidence for the identification of admixed components and to check that no other separable components were present. III and IV were identified as the principle constituents of the trimethylsilylated cryst. fraction of a natural glycoside ext. by gas and chromatographic anal. on an OV-17 column and by ir and uv spectroscopy.
 IT 19764-02-4
 RL: ANT (Analyte); ANST (Analytical study)
 (detn. of, chromatographic)
 RN 19764-02-4 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

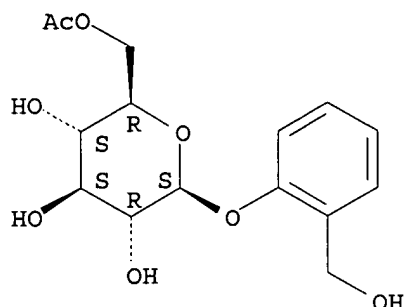
Absolute stereochemistry.



L4 ANSWER 22 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1968:454269 CAPLUS
 DOCUMENT NUMBER: 69:54269
 TITLE: Determination of phenolic glycosides in some domestic Salix species
 AUTHOR(S): Kytkowska, Otylia
 CORPORATE SOURCE: Inst. Lekow, Warsaw, Poland
 SOURCE: Herba Pol. (1967), 13(4), 177-83
 CODEN: HPBIA9

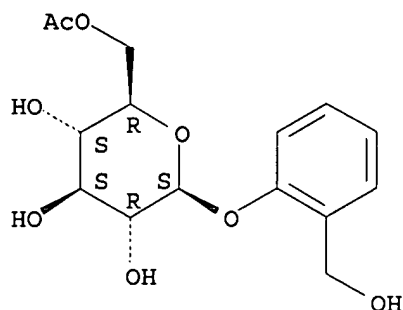
DOCUMENT TYPE: Journal
 LANGUAGE: Polish
 AB Combined EtOH and H₂O exts. from barks of each of 7 *Salix* species (*S. purpurea*, *S. alba*, *S. viminalis*, *S. caprea*, *S. cinerea*, *S. fragilis*, and *S. cordata*) were evapd. in vacuo, extd. with EtOAc, and sepd. by paper chromatog. The samples contained salicin, triandrin, fragilin, salicortin, picein, vimalin, and salireposide. The triandrin levels were 0.45-5.35%, and those of salicortin, 0.05-4.8%.
 IT 19764-02-4
 RL: ANT (Analyte); ANST (Analytical study)
 (detn. of, in *Salix* species)
 RN 19764-02-4 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1968:436405 CAPLUS
 DOCUMENT NUMBER: 69:36405
 TITLE: The barks of the family Salicaceae. XV. The leaves of the family Salicaceae. 10. Mass spectrometry as an aid for determining structures of natural glucosides
 AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
 CORPORATE SOURCE: Inst. of Paper Chem., Appleton, Wis., USA
 SOURCE: Phytochemistry (1968), 7(5), 831-7
 CODEN: PYTCAS
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Mass spectral fragmentation patterns were detd. for acetates of a no. of glucosides of unequivocally known structure which were isolated from the barks and leaves of trees of the family Salicaceae. All glucoside acetates, irrespective of size, indicated primary fragmentation at the C-1 bond, essentially similar to that found for completely acetylated glucose and methyl glucoside. In addn., the spectra of the acetates of glucosides with free phenolic groups demonstrated loss of acetyl as ketene either concurrently with or before the rupture of the C-1 bond. Presence or absence of ester substitution in the glucose moiety of the parent glucosides could thus be detd. with certainty, and possible location of substitution is indicated by relative intensities of fragment peaks.
 IT 19764-02-4
 RL: PRP (Properties)
 (mass spectrum of)
 RN 19764-02-4 CAPLUS
 CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 24 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:514359 CAPLUS

DOCUMENT NUMBER: 67:114359

TITLE: Barks of the family Salicaceae. XIII. Hot-water

extractives of the green bark of *Populus trichocarpa*

AUTHOR(S): Estes, Timothy K.; Pearl, Irwin A.

CORPORATE SOURCE: Inst. of Paper Chem., Appleton, Wis., USA

SOURCE: Tappi (1967), 50(7), 318-24

CODEN: TAPPAP

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

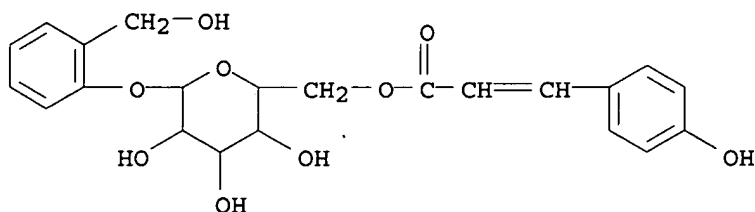
AB cf. CA 65: 9006c. The oven-dry ground bark of *P. trichocarpa* (1.5 kg.) was extd. with 20 l. hot H₂O, the ext. filtered over Celite, and concd. in vacuo to .apprx.2 l. contg. 16% of the bark. The ext. was exhaustively extd. with CHCl₃, Et₂O, and EtOAc, giving the extractives I (8%), II (10%), and III (20%), resp. The final raffinate (IV) contained 62% of the hot H₂O extractives. I was triturated with EtOH and the waxy residue discarded. I was then sepd. with Pb subacetate into 17% of a "Pb-sol." fraction, Ia, and 49% of a "Pb-insol." fraction, Ib. By polyamide chromatog. (P.C.) of Ia, salicin (V), salicyl alc. (VI), and tremuloidin (VII) and a mixt. of trichocarpin (VIII) and salireposide (IX) were isolated. P.C. of Ib indicated the presence of pyrocatechol, V, VI, VIII, and IX. Acid hydrolysis of I gave no salicyloylsalicin deriv. P.C. of II gave VIII, IX, p-coumaric acid (X), and trichocarposide (XI), m. 180-2.degree. (H₂O), [.alpha.]_D²⁰ -11.4.degree. (c 2.3, 80% Me₂CO). Pb subacetate treatment of II gave VIII, IX, X, and XI. Pb subacetate and P.C. of II gave VIII, IX, X, and XI. Mild hydrolysis and P.C. of III indicated the presence of salicyloylsalicin-2 benzoate and X. P.C. of IV indicated the presence of glucose, fructose, and sucrose. Alk. hydrolysis of XI gave III and X; periodate oxidn. of XI consumed 2 moles with the liberation of 1 mole HCO₂H. Hydrolysis of XI with .beta.-glucosidase gave no glucose. 21 references.

IT 17063-94-4

RL: BIOL (Biological study)
(from *Populus trichocarpa* bark)

RN 17063-94-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-[3-(4-hydroxyphenyl)-2-propenoate] (9CI) (CA INDEX NAME)



L4 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1964:462667 CAPLUS
DOCUMENT NUMBER: 61:62667
ORIGINAL REFERENCE NO.: 61:10918e-f
TITLE: Isolation of methoxyeugenol and trans-isoelemicin from the oil of nutmeg
AUTHOR(S): Shulgin, A. T.; Kerlinger, H. O.
CORPORATE SOURCE: Dow Chem. Co., Walnut Creek, CA
SOURCE: Naturwissenschaften (1964), 51(15), 360-1
DOCUMENT TYPE: Journal
LANGUAGE: English

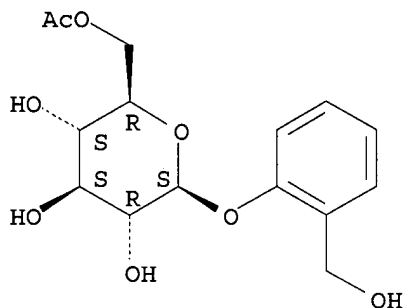
AB Fractional distn. of oil of nutmeg gave 3 fractions. Fraction A cuts up to 114.degree. at 2 mm. consisted of terpenes, fraction B 114-119.degree. at 2 mm. contained myristicin (I) and elemicin (II), fraction C was a heavy oil residue which contained I and II as well as methoxyeugenol (III) and transisoelemicin (IV). Nuclear magnetic resonance, infrared, and mixed m.p. of the benzoate deriv. of III confirmed its identity. IV was confirmed by infrared and its dibromo deriv. A search for trans-isomyristicin and the methoxylated analog revealed only extremely small traces.

IT 19764-02-4, Salicin, 6'-acetate
(identity with fragilin from willow)

RN 19764-02-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1964:462666 CAPLUS
DOCUMENT NUMBER: 61:62666
ORIGINAL REFERENCE NO.: 61:10918d-e
TITLE: The constitution of fragilin
AUTHOR(S): Thieme, H.
CORPORATE SOURCE: Univ. Leipzig, Germany
SOURCE: Naturwissenschaften (1964), 51(13), 310
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

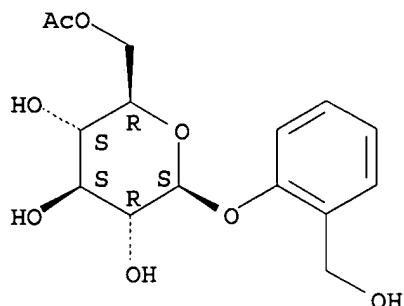
AB Fragilin (a new phenol-glucoside from *Salix fragilis*) was permethylated with MeI and Ag₂O in dimethylformamide. Paper chromatographic examination showed the presence of 2,3,4-trimethylglucose, from which it was decided that fragilin is 6-acetylsalicin.

IT 19764-02-4, Salicin, 6'-acetate
(identity with fragilin from willow)

RN 19764-02-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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86110 ESTERIFICATION

437 ESTERIFICATIONS

86235 ESTERIFICATION

(ESTERIFICATION OR ESTERIFICATIONS)

L6 3 L4 AND ESTERIFICATION

=> d l6 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:472959 CAPLUS

DOCUMENT NUMBER: 135:75834

TITLE: Enzyme-catalysed modification of substances in biological mixtures

INVENTOR(S): Otto, Ralf; Weiss, Albrecht

PATENT ASSIGNEE(S): Cognis Deutschland G.m.b.H., Germany

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046452	A1	20010628	WO 2000-EP12652	20001213
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
DE 19962204	A1	20010705	DE 1999-19962204	19991222
EP 1240349	A1	20020918	EP 2000-987394	20001213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				

PRIORITY APPLN. INFO.: DE 1999-19962204 A 19991222

WO 2000-EP12652 W 20001213

AB The invention relates to an enzyme-catalyzed modification of substances in a mixt., comprising bringing the substance in a mixt. to be modified into contact with an enzyme and a substrate. Thus, arbutin present in a com. leaf ext. of bearberry was mixed with palmitic acid in the presence of an immobilized lipase and incubated at 45 .degree.C for 24 h. The resulting palmitoyl arbutin was then extd. with chloroform or methylene chloride.

IT 270081-79-3P

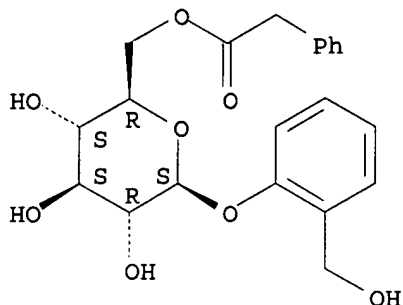
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(enzyme-catalyzed modification of compds. in biol. exts.)

RN 270081-79-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI)

(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:393069 CAPLUS

DOCUMENT NUMBER: 131:43666

TITLE: Method for selective **esterification** of polyols

INVENTOR(S): Otto, Ralf; Syldatk, Christoph; Cao, Linqiu; Bornscheuer, Uwe; Schmid, Rolf D.

PATENT ASSIGNEE(S): Henkel K.-G.a.A., Germany

SOURCE: Ger. Offen., 8 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19753789	A1	19990617	DE 1997-19753789	19971204

OTHER SOURCE(S): CASREACT 131:43666; MARPAT 131:43666

AB The prodn., from the corresponding polyol and carboxylic acid contg. an arom. ring, of polyols esterified on the primary -OH group is improved in selectivity and yield without introducing and removing protecting groups. This is characterized in that the polyol and carboxylic acid, in the presence of a small amt. of org. solvent that dissolves neither completely, react with each other under catalysis by a lipase or an esterase. The products have emulsifying activity with potential pharmaceutical use.

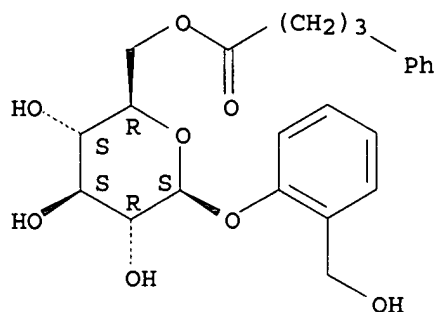
IT 218966-96-2P

RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(selective **esterification** of polyols)

RN 218966-96-2 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:52346 CAPLUS

DOCUMENT NUMBER: 108:52346

TITLE: Protease-catalyzed regioselective
esterification of sugars and related compounds
in anhydrous dimethylformamide

AUTHOR(S): Riva, Sergio; Chopineau, Joel; Kieboom, A. P. G.;
Klibanov, Alexander M.

CORPORATE SOURCE: Dep. Appl. Biol. Sci., Massachusetts Inst. Technol.,
Cambridge, MA, 02139, USA

SOURCE: Journal of the American Chemical Society (1988),
110(2), 584-9

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

AB By taking advantage of the unique dissolving potency of DMF and the broad substrate specificity of subtilisin, a no. of carbohydrates and other sugar-contg. compds. were regioselectively acylated via enzymic transesterification. Monobutyl esters of the disaccharides maltose, cellobiose, lactose, and sucrose were prepd. readily on a gram scale. The presence of a bulky aglycon moiety does not substantially reduce the catalytic efficiency of subtilisin in DMF, thus permitting preparative enzymic **esterification** of natural compds. such as riboflavin, salicin, and the nucleosides adenosine and uridine. The reactivity of subtilisin only modestly drops upon an increase in the size of the carbohydrate substrate from maltose to maltoheptose. In addn. to the butyl group, various N-acetylamino acid residues were enzymically introduced into sugars. Both highly purified and crude preps. of subtilisin were used successfully as practical catalysts of transesterifications in dry DMF.

IT 111933-84-7P

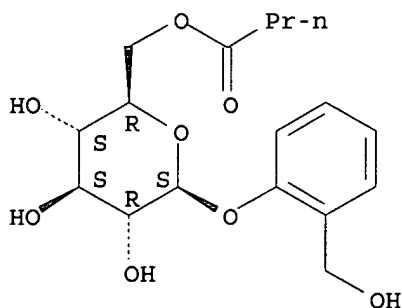
RL: PREP (Preparation)

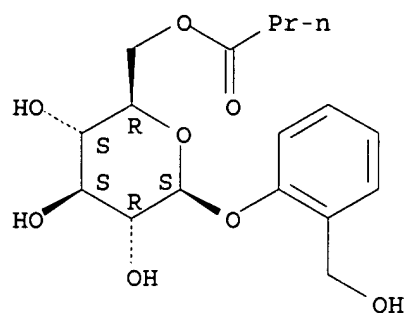
(prepn. of, by **esterification** of subtilisin in anhyd. DMF)

RN 111933-84-7 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-butanoate (9CI) (CA
INDEX NAME)

Absolute stereochemistry.





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(FILE 'HOME' ENTERED AT 12:59:38 ON 01 DEC 2002)

FILE 'REGISTRY' ENTERED AT 12:59:46 ON 01 DEC 2002

L1 STRUCTURE UPLOADED

L2 0 S L1 SSS SAM

L3 10 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 13:01:55 ON 01 DEC 2002

L4 26 S L3

L5 26 DUP REM L4 (0 DUPLICATES REMOVED)

L6 3 S L4 AND ESTERIFICATION

s 14 and prostaglandin

60913 PROSTAGLANDIN

39884 PROSTAGLANDINS

69447 PROSTAGLANDIN

(PROSTAGLANDIN OR PROSTAGLANDINS)

L7 1 L4 AND PROSTAGLANDIN

=> d 17 1 ibib abs hitstr

L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:472959 CAPLUS

DOCUMENT NUMBER: 135:75834

TITLE: Enzyme-catalysed modification of substances in biological mixtures

INVENTOR(S): Otto, Ralf; Weiss, Albrecht

PATENT ASSIGNEE(S): Cognis Deutschland G.m.b.H., Germany

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046452	A1	20010628	WO 2000-EP12652	20001213
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
DE 19962204	A1	20010705	DE 1999-19962204	19991222
EP 1240349	A1	20020918	EP 2000-987394	20001213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				

PRIORITY APPLN. INFO.: DE 1999-19962204 A 19991222

WO 2000-EP12652 W 20001213

AB The invention relates to an enzyme-catalyzed modification of substances in a mixt., comprising bringing the substance in a mixt. to be modified into contact with an enzyme and a substrate. Thus, arbutin present in a com. leaf ext. of bearberry was mixed with palmitic acid in the presence of an immobilized lipase and incubated at 45 .degree.C for 24 h. The resulting palmitoyl arbutin was then extd. with chloroform or methylene chloride.

IT 270081-79-3P

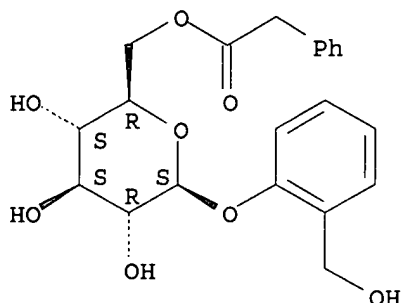
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)

(enzyme-catalyzed modification of compds. in biol. exts.)

RN 270081-79-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s l4 and inhibition of prostaglandin

650067 INHIBITION
4491 INHIBITIONS
651545 INHIBITION
(INHIBITION OR INHIBITIONS)
60913 PROSTAGLANDIN
39884 PROSTAGLANDINS
69447 PROSTAGLANDIN
(PROSTAGLANDIN OR PROSTAGLANDINS)
2087 INHIBITION OF PROSTAGLANDIN
(INHIBITION(1W) PROSTAGLANDIN)

L8 0 L4 AND INHIBITION OF PROSTAGLANDIN

=> s l4 and prostaglandin(w) synthesis

60913 PROSTAGLANDIN
39884 PROSTAGLANDINS
69447 PROSTAGLANDIN
(PROSTAGLANDIN OR PROSTAGLANDINS)
1033831 SYNTHESIS
2 SYNTHESISES
57799 SYNTHESSES
1067671 SYNTHESIS
(SYNTHESIS OR SYNTHESISES OR SYNTHESSES)
5951 PROSTAGLANDIN(W) SYNTHESIS

L9 0 L4 AND PROSTAGLANDIN(W) SYNTHESIS

L11 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:403512 CAPLUS
 DOCUMENT NUMBER: 111:3512
 TITLE: The effect of the sample **preparation** method of extractable phenolics of Salicaceae species
 AUTHOR(S): Julkunen-Tiitto, R.; Tahvanainen, J.
 CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, SF-80101, Finland
 SOURCE: Planta Medica (1989), 55(1), 55-8
 CODEN: PLMEAA; ISSN: 0032-0943
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The effect of different tissue prehandling methods on the phenolic content of willow bark, leaves, and twigs was studied. The phenolics were extd. at room temp., purified, and analyzed by high-resoln. capillary gas chromatog. Neither oven drying at a low temp. nor room drying of fresh leaves and oven drying of bark produced any qual. changes in the glucoside compn. and only a minor binding effect was seen on the amts. of each glucoside. On the other hand, oven drying of the intact long twigs and room drying of the bark are prehandling methods to avoid. Freeze drying or immediate anal. of frozen leaves lowered the total amt. of glucosides and caused considerable qual. changes to the glucoside compn. Acetone (80%) was a slightly more effective and gentle extn. solvent for all glucosides compared with methanol.

L11 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:489072 CAPLUS
 DOCUMENT NUMBER: 109:89072
 TITLE: Comparative high-performance liquid and gas-liquid chromatographic determination of phenolic glucosides in Salicaceae species
 AUTHOR(S): Meier, B.; Julkunen-Tiitto, R.; Tahvanainen, J.; Sticher, O.
 CORPORATE SOURCE: Dep. Pharm., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.
 SOURCE: Journal of Chromatography (1988), 442, 175-86
 CODEN: JOCRAM; ISSN: 0021-9673
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The phenolic glucosides of 7 willow species with different glucoside patterns were extd., purified, and analyzed by GC and HPLC. Two sample **prepn.** methods were used. It was shown that the HPLC and GC methods give comparable qual. and quant. results for the phenolic glucoside contents of the tested willows. Consequently, both methods can be used for species-specific screening of the glucoside patterns of Salicaceae species.

L11 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1970:78749 CAPLUS
 DOCUMENT NUMBER: 72:78749
 TITLE: Minor anthraquinones of Xanthoria parietina, the chlorination of parietin,, and the synthesis of **fragilin** and 7-chloroemodin ("AO-1")
 AUTHOR(S): Sargent, Melvyn V.; Smith, David O'N.; Elix, J. A.
 CORPORATE SOURCE: Univ. Chem. Lab., Canterbury, Engl.
 SOURCE: J. Chem. Soc. C (1970), (2), 307-11
 CODEN: JSOOAX
 DOCUMENT TYPE: Journal
 LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Extn. of the lichen X. parietina yielded the anthraquinones emodin, teloschistin, and parietinic acid, as well as parietin (I). Chlorination of I with chlorine (1 mole) gave 5-chloroparietin, with chlorine (2 mole) gave chiefly 4,5-dichloroparietin, and with

excesschlorine gave 4,5,7-trichloroparietin (II). Dechlorination of II with excess sodium dithionite gave I and with a deficiency of sodium dithionite gave, after methylation, tri-O-methylemodin and 4,5,7-trichlorodi-O-methylparietin. Dechlorination of II with hydrazine hydrate and Pd/C after methylation, furnished di-O-methylfragilin III). Partial demethylation of III yielded **fragilin**, and complete demethylation of the former compd. afforded 7-chloroemodin.

L11 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1966:5478 CAPLUS
DOCUMENT NUMBER: 64:5478
ORIGINAL REFERENCE NO.: 64:1013c-d
TITLE: The phenolic glycosides of Salicaceae. V. Glycoside spectra and glycosidic content of Salix species of central Germany
AUTHOR(S): Thieme, Heinz
CORPORATE SOURCE: Karl Marx Univ., Leipzig, Germany
SOURCE: Pharmazie (1965), 20(9), 570-4
DOCUMENT TYPE: Journal
LANGUAGE: German

AB cf. CA 63, 11685g. Leaves, inflorescences, and barks of 11 willow spp. were studied, with sepn. wherever possible on the basis of sex. Paper chromatography, after preliminary purification of the exts. by passage through polyamide columns, was used to sep. the various glycosides isolated; they were identified by cochromatography or by elution and detn. of m.ps. or mixed m.ps. Glycosidal compn. was highly variable; salicin (I) (regarded as the chief glycoside of the Salicaceae) was detectable in all barks studied but was present only in small concns. and never was the chief glycoside. Larger amts. of acylated I derivs. were observed in various species; esp. high concns. of salicortin (II) or of triandrin were contained in barks of Salix purpurea or S. viminalis collected in mid-March. In contrast to the barks, leaves and inflorescences did not always contain phenol glycosides. The leaves of a few species; (S. myrsinifolia, S. purpurea, S. repens) evidenced noteworthy high concns. of I and II. No significant relation of glycoside content to sex of plant could be established. 27 references.

L11 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1965:438909 CAPLUS
DOCUMENT NUMBER: 63:38909
ORIGINAL REFERENCE NO.: 63:6930e-g
TITLE: The constitution of **fragilin**
AUTHOR(S): Bruun, Torger; Hollis, Donald P.; Ryhage, Ragnar
CORPORATE SOURCE: Norges Tek. Hogskole, Trondheim, Norway
SOURCE: Acta Chem. Scand. (1965), 19(4), 839-44
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB **Fragilin** (I) is a minor, colored constituent of the lichens Sphaerophorus fragilis (II) and S. coralloides. I was obtained from II and from S. globosus by extg. with ether for 24 hrs. The exts. were concd. and extd. successively with NaHCO₃, Na₂CO₃, and NaOH. The org. material in the NaOH ext. was liberated with dil. H₂SO₄ and extd. with ether. After removal of the ether, an oil was recovered which gradually solidified and crystd. The crystals were isolated with ether or CHCl₃ and purified by fractionated sublimation under reduced pressure and/or by crystn. from CHCl₃, m. 267-8.degree.. Based on high resolution N.M.R. and mass spectroscopy, I was given the constitution below. The methoxy deriv. was obtained by methylation with Me₂SO₄ and K₂CO₃ in acetone, the yellow crystals were recovered from CHCl₃-MeOH, m.p. 208-9.degree.. Acetylation with acetic anhydride in pyridine, overnight at room temp. yielded the acetate, the yellow crystals were recovered from acetone, m. 234-5.degree..

L5 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:727039 CAPLUS

DOCUMENT NUMBER: 137:252711

TITLE: Melanin formation promoting agents containing salicylic acid or **salicyl** alcohol derivatives

INVENTOR(S): Hasegawa, Junichi; Tanaka, Kiyotaka

PATENT ASSIGNEE(S): Ichimaru Pharcos Inc., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 30 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002275060	A2	20020925	JP 2001-75402	20010316

OTHER SOURCE(S): MARPAT 137:252711

AB The invention relates to a melanin formation promoting agent suitable for use in a cosmetic compn. for rough skin improvement and hair growth stimulation, etc., wherein the melanin formation promoting agent contains a salicylic acid or **salicyl** alc. deriv. A cosmetic emulsion contg. 2-hydroxybenzoylaminoacetate 0.1 % was prepd.

IT 138-52-3

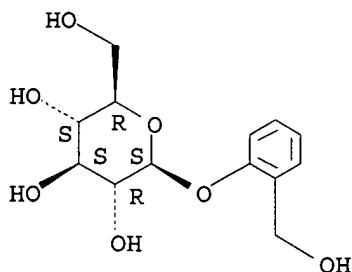
RL: COS (Cosmetic use); PAC (Pharmacological activity); BIOL (Biological study); USES (Uses)

(melanin formation promoting agents contg. salicylic acid or **salicyl** alc. derivs.)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:521356 CAPLUS

DOCUMENT NUMBER: 137:75540

TITLE: Methods for generating doubled haploid maize plants

INVENTOR(S): Zheng, Yuanming; Konzak, Calvin F.; Weng, Yujia; Rafiullah, Sahibzada

PATENT ASSIGNEE(S): Northwest Plant Breeding Co., USA

SOURCE: PCT Int. Appl., 37 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2002052926 A2 20020711 WO 2002-US327 20020102

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-260028P P 20010105

AB In one aspect, the present invention provides methods for generating doubled haploid and/or haploid maize plants from microspores. The methods of this aspect of the invention include the steps of: (a) selecting maize plant material comprising maize microspores at a developmental stage amenable to androgenic induction; (b) incubating the microspores in incubation medium at a temp. and osmolarity effective to induce androgenesis to obtain temp.-treated microspores; (c) isolating the temp.-treated microspores; (d) cultivating the isolated, temp.-treated microspores in cultivation medium with either at least one live plant ovary and/or ovary-conditioned medium to produce regenerative maize tissue, wherein the cultivation medium has an osmolarity between about 300 mOsm and about 500 mOsm and comprises at least one cytokinin and at least one auxin; and (e) regenerating maize plants from the regenerative maize tissue. The present invention also provides methods for producing regenerative maize tissue from maize microspores.

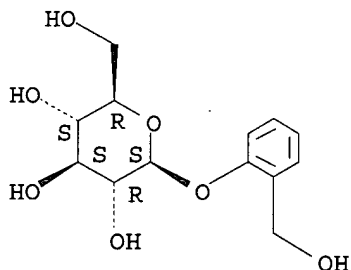
IT 138-52-3, Salicin

RL: BSU (Biological study, unclassified); BIOL (Biological study) (methods for generating doubled haploid maize plants)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:405294 CAPLUS

DOCUMENT NUMBER: 137:43683

TITLE: Determination of triandrin and salicin in *Salix viminalis* L. by reversed-phase high-performance liquid chromatography

AUTHOR(S): Minakhmetov, R. A.; Onuchak, L. A.; Kurkin, V. A.; Zapesochaya, G. G.; Medvedeva, S. A.

CORPORATE SOURCE: Department of Chemistry, Samara State University, Samara, 443011, Russia

SOURCE: Journal of Analytical Chemistry (Translation of Zhurnal Analiticheskoi Khimii) (2002), 57(4), 338-341
CODEN: JACTE2; ISSN: 1061-9348

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The optimal sepn. of phenolic components of the bark of basket willow *Salix viminalis* L. was attained using reversed-phase HPLC with isocratic elution. Triandrin (1-O-.beta.-D-glucopyranoside of p-coumaryl alc.) and salicin (1-O-.beta.-D-glucopyranoside of salicyl alc.) were identified. Regularities in the retention of triandrin and salicin in the Separon SGX C18-binary mobile phase (acetonitrile-H₂O) system were considered. A procedure was developed for the quant. detn. of triandrin in raw basket-willow bark and its ext.

IT 138-52-3, Salicin

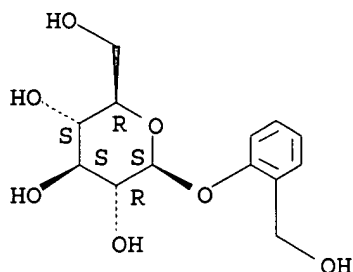
RL: ANT (Analyte); ANST (Analytical study)

(detn. of triandrin and salicin in *Salix viminalis* L. by reversed-phase high-performance liq. chromatog.)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:85522 CAPLUS

DOCUMENT NUMBER: 136:276441

TITLE: Functional expression of human liver cytosolic .beta.-glucosidase in *Pichia pastoris*. Insights into its role in the metabolism of dietary glucosides
AUTHOR(S): Berrin, Jean-Guy; McLauchlan, W. Russell; Needs, Paul; Williamson, Gary; Puigserver, Antoine; Kroon, Paul A.; Juge, Nathalie

CORPORATE SOURCE: Nutrition, Health and Consumer Sciences Division, Institute of Food Research, Norwich, NR4 7UA, UK

SOURCE: European Journal of Biochemistry (2002), 269(1), 249-258

CODEN: EJBCAI; ISSN: 0014-2956

PUBLISHER: Blackwell Publishing Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Human tissues such as liver, small intestine, spleen and kidney contain a cytosolic .beta.-glucosidase (CBG) that hydrolyzes various .beta.-D-glycosides, but whose physiol. function is not known. Here, we describe the first heterologous expression of human CBG, a system that facilitated a detailed assessment of the enzyme specificity towards dietary glycosides. A full-length CBG cDNA (cbg-1) was cloned from a human liver cDNA library and expressed in the methylotrophic yeast *Pichia pastoris* at a secretion yield of .apprx.10 mg/L. The recombinant CBG (reCBG) was purified from the supernatant using a single chromatog. step and was shown to be similar to the native enzyme isolated from human liver in terms of phys. properties and specific activity towards 4-nitrophenyl-.beta.-D-glucoside. Furthermore, the reCBG displayed a broad specificity with respect to the glycone moiety of various aryl-glycosides (.beta.-D-fucosides, .alpha.-L-arabinosides, .beta.-D-glucosides, .beta.-D-galactosides, .beta.-L-xylosides,

.beta.-D-arabinosides), similar to the native enzyme. For the first time, we show that the human enzyme has significant activity towards many common dietary xenobiotics including glycosides of phytoestrogens, flavonoids, simple phenolics and cyanogens with higher apparent affinities (K_m) and specificities (k_{cat}/K_m) for dietary xenobiotics than for other aryl-glycosides. These data indicate that human CBG hydrolyzes a broad range of dietary glucosides and may play a crit. role in xenobiotic metab.

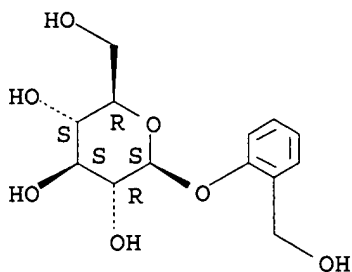
IT 138-52-3, Salicin

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(functional expression of human liver cytosolic .beta.-glucosidase and its role in metab. of dietary glucosides in *Pichia pastoris*)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:724753 CAPLUS

DOCUMENT NUMBER: 136:17988

TITLE: Glycosides of benzyl and salicyl alcohols
from *Alangium chinense*

AUTHOR(S): Itoh, Atsuko; Tanahashi, Takao; Nagakura, Naotaka;

Inoue, Kenichiro; Kuwajima, Hiroshi; Wu, Hua-Xin

CORPORATE SOURCE: Kobe Pharmaceutical University, Kobe, 658-8558, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (2001), 49(10),
1343-1345

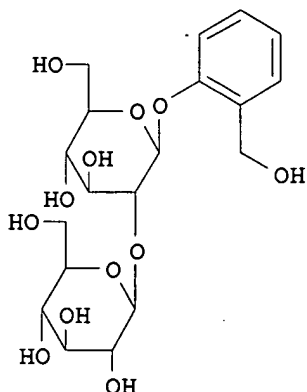
CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB From the water-sol. fraction of the dried leaves of *Alangium chinense*, three new glycosides, benzyl alc. .beta.-D-glucopyranosyl-(1.fwdarw.2)-[.beta.-D-xylopyranosyl-(1.fwdarw.6)]-.beta.-D-glucopyranoside, 2'-O-.beta.-D-glucopyranosylsalicin (I), and 2'-O-.beta.-D-glucopyranosyl-6'-O-.beta.-D-xylopyranosylsalicin were isolated along with seven known glycosides. The structures of the new compds. were detd. by spectroscopic and chem. means.

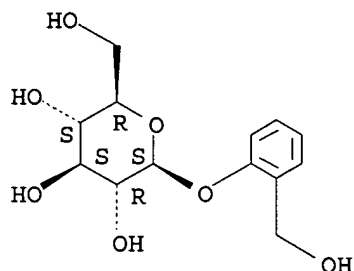
IT 138-52-3, Salicin 72021-23-9, Henryoside
193280-03-4, 6'-O-.beta.-D-Xylopyranosylsalicin

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(glycosides of benzyl and **salicyl** alcs. from *Alangium chinense*)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

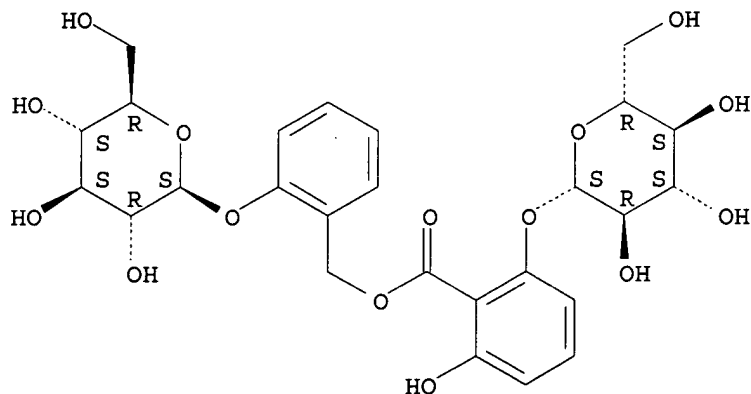
Absolute stereochemistry.



RN 72021-23-9 CAPLUS

CN .beta.-D-Glucopyranoside, 2-[[[2-(.beta.-D-glucopyranosyloxy)-6-hydroxybenzoyl]oxy]methyl]phenyl (9CI) (CA INDEX NAME)

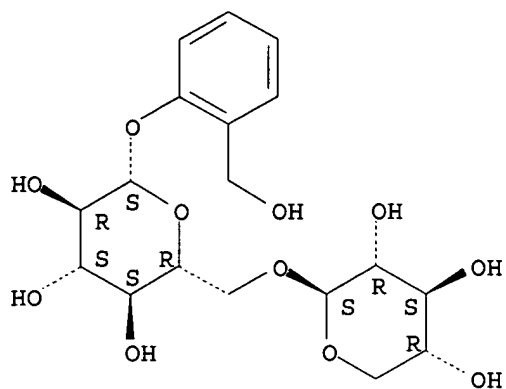
Absolute stereochemistry.



RN 193280-03-4 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl 6-O-.beta.-D-xylopyranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 377086-35-6P 377086-36-7P

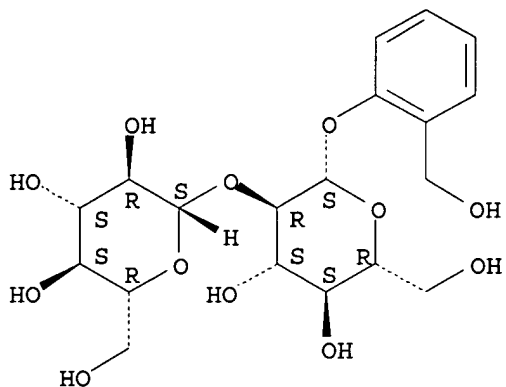
RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(glycosides of benzyl and **salicyl** alcs. from *Alangium chinense*)

RN 377086-35-6 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl 2-O-.beta.-D-glucopyranosyl- (9CI) (CA INDEX NAME)

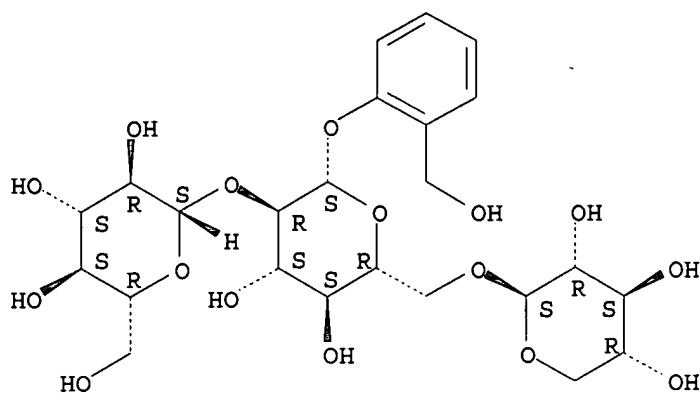
Absolute stereochemistry.



RN 377086-36-7 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl O-.beta.-D-glucopyranosyl-(1.fwdarw.2)-O-[.beta.-D-xylopyranosyl-(1.fwdarw.6)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:560508 CAPLUS

DOCUMENT NUMBER: 135:288062

TITLE: Does excretion of secondary metabolites always involve a measurable metabolic cost? Fate of plant antifeedant salicin in common brushtail possum, *Trichosurus vulpecula*

AUTHOR(S): McLean, S.; Pass, G. J.; Foley, W. J.; Brandon, S.; Davies, N. W.

CORPORATE SOURCE: School of Pharmacy, University of Tasmania, Hobart, 7001, Australia

SOURCE: Journal of Chemical Ecology (2001), 27(6), 1077-1089
CODEN: JCECD8; ISSN: 0098-0331

PUBLISHER: Kluwer Academic/Plenum Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Salicin was given to 6 brushtail possums in diet for 6 days at 0.05, 0.5, and 1.5% feed wet wt. (mean daily intakes 0.31+-0.09, 2.76+-0.75, and 6.04+-1.12 mmol salicin, resp.). Salicin metabolites were analyzed by HPLC and MS. **Salicyl alc.** glucuronide accounted for 56-64% of urinary metabolites over the 3 doses, salicyluric acid 15-26%, and salicin 10-18%; there were smaller amts. of free (2-4%) and conjugated (0-6%) salicylic acid. The **.beta.,2-dihydroxyphenylpropionic acid** was a minor metabolite. Hydrolysis of the dietary salicin allowed reconjugation of its aglycon, **salicyl alc.**, with a more polar sugar, glucuronic acid, thus enhancing its renal excretion and leading to small net loss of substrates for conjugation and low measurable metabolic costs of excretion.

IT 138-52-3, Salicin

RL: BPR (Biological process); BSU (Biological study, unclassified); FFD (Food or feed use); BIOL (Biological study); PROC (Process); USES (Uses) (dietary salicin plant antifeedant compd. intake and metabolic cost of its urinary metabolites excretion in common brushtail possum (*Trichosurus vulpecula*))

RN 138-52-3 CAPLUS

CN **.beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI)** (CA INDEX NAME)

Absolute stereochemistry.

SYNTHESIS OF IMIDAZO[1,2-c]PYRIMIDINE DERIVATIVES

Florentina Georgescu,³ Emilian Georgescu,³ Paula C. Iuhas,³ Constantin Draghici,³ Miron Caproiu,^b Petru I. Filip^b a. S. C. OLTCHIM S. A.-Research

Center, 1 Uzinei St., 1000 Ramnicu Valcea, Romania;

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b. Romanian Academy-Center for Organic Chemistry, Spl. Independentei 202B, 77208 Bucharest, Romania

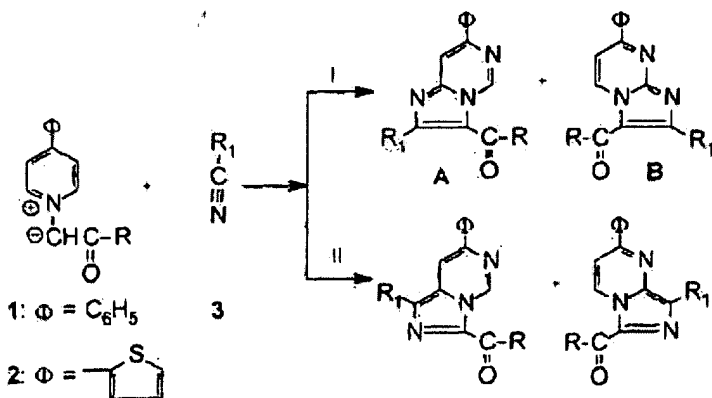
Introduction

Imidazo[1,2-c]pyrimidine derivatives have interesting chemical and biological properties, which raised up numerous studies.¹⁻⁴ In this field we are particularly interested in the synthesis of imidazo[1,2-c]pyrimidine derivatives with potential biological activities.

The common methods for the synthesis of imidazo-azines are based on the condensation reactions: the condensation of heterocyclic amines with α -halocarbonyl compounds^{1,3}, the reaction of α -aminoheterocyclic compounds with 1,2-dibromoethane followed by oxidation⁴, or the reaction of chloroazines with α -aminoacetaldehyde diethyl acetal^{4,5}. An interesting method for the synthesis of imidazo-azines is based on 1,3-dipolar cycloaddition reactions of cycloimmonium-ylides with dipolarophile compounds containing activated carbon-nitrogen triple bond. This method was applied for the synthesis of imidazo[1,2-a]pyridine and imidazo[2,1-b]isoquinoline derivatives by the 1,3-dipolar cycloaddition reactions of pyridinium- and isoquinolinium-ylides with trifluoroacetonitrile⁶. Only one imidazo[1,2-a]pyrimidine, with very poor yield, was obtained by this method. Herein, we present new imidazo[1,2-a]pyrimidine derivatives obtained by 1,3-dipolar cycloaddition reactions of 4-substituted pyrimidinium-ylides with dipolarophile compounds containing activated carbon-nitrogen triple bond such as trifluoroacetonitrile and benzoyl cyanide.

Results and Discussion

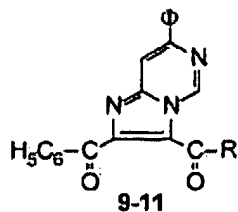
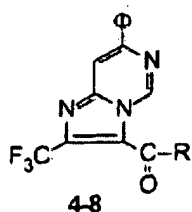
Theoretically, in the [3+2] dipolar cycloaddition reactions of 4-substituted pyrimidinium-ylides with unsymmetrical substituted carbon-nitrogen triple bond compounds the following regioisomers A-C could be obtained (scheme 1).



Scheme 1. The four possible regioisomers in the [3+2] dipolar cycloadditions of 4-substituted pyrimidinium-ylides to carbon-nitrogen triple bond compounds.

By the reactions of several 4-substituted pyrimidinium-ylides 1, and respectively 2, to trifluoroacetonitrile 3a ($\text{R}_1 = \text{CF}_3$), and respectively benzoyl cyanide 3b ($\text{R}_1 = \text{C}_6\text{H}_5$), only one type of each trifluoromethyl-substituted imidazo[1,2-c]pyrimidines 4-8, respectively benzoyl-substituted imidazo[1,2-c]pyrimidines 9-11, were obtained (scheme 2). The 4-substituted pyrimidinium-ylides were generated *in situ* from the corresponding quaternary salts in the presence of an acid acceptor such as triethylamine or 1,2-epoxybutane.^{7,10}

New prepared 5-trifluoromethyl- and 5-benzoyl-pyrrolo[1,2-c]pyrimidine derivatives 4-11 (scheme 1) were characterised by melting points, IR and NMR spectroscopy. IR and NMR data confirm the A-type structure of the obtained cycloadducts 4-11.



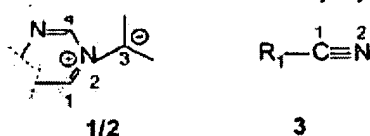
Comp.	o>	R	m.p. (°C)	Yield (%)	4	C ₆ H ₅
C ₆ H ₅	197-198.5	30.2 5	C ₆ H ₅	C ₆ H ₄ F(pJ)	198-201	
29.4 6	C ₆ H ₅	C ₆ H ₄ OCH ₃ (pJ)	173-176	28.2 7	C ₆ H ₆	
C ₆ H ₄ NO ₂ (pJ)	248-251	34.5 8	2-thienyl	C ₆ H ₃ (3,4-OCH ₃) ₂	239-241	
30.0 9	C ₆ H ₅	C ₆ H ₅	215-217	29.4 10	C ₆ H ₅	
C ₆ H ₄ NO ₂ (pJ)	242-244	34.2 11	2-thienyl	C ₆ H ₃ (3,4-OCH ₃) ₂	230-234	
30.6						

Scheme 2. New synthesized imidazo[1,2-c]pyrimidines

A theoretical study concerning the regiochemistry of cycloaddition reactions of 4-substituted pyrimidinium-ylides as 1,3-dipoles to trifluoroacetonitrile and benzoyl cyanide as dipolarophiles was performed to explain the regioselectivity. We have used the General Theory of Perturbation of the Molecular Frontier Orbitals^{11,12}.

The energies (eV) of frontier molecular orbitals (HOMO and LUMO), the coefficients of atomic orbital p_z and the total atomic charges (in coulombs) for all the atoms involved in the cycloaddition reactions of pyrimidinium-ylides **1a** and **2a** to trifluoroacetonitrile **3a**, respectively benzoyl cyanide **3b**, are presented in Table 1.

Table 1. Atomic charges, atomic orbital coefficients and frontier molecular orbital energies of ylides **1a** and **2a**, trifluoroacetonitrile **3a** and benzoyl cyanide **3b**.



Frontier orbitals	Orbital Molecule	molecular	energy	C-1	N-2	C-3	C-4
Ylidela	HOMO	-7.78297	+0.33413	+0.07110	-0.65444	+0.33643	<D=C ₆ H ₅ , Q
LUMO	-1.24434	+0.26000	-0.44268	-0.30670	+0.19343	R=C ₆ H ₅	
-0.160	+0.142	-0.404	-0.082	Ylide2a	HOMO	-7.7755	+0.3084
+0.0699	-0.6209	+0.3234	<X>=2-thienyl,	LUMO	-1.3153	-0.1736	+0.4041
0.2969	-0.2226	R=C ₆ H ₄ (3,4-Q			-0.135	+0.142	-0.412
0.104	OCH ₃) ₂ 3a	HOMO	-14.18754	+0.34271	-0.38373	(Ri=CF ₃)	LUMO
+0.35250	-0.26350	+0.27280	Q		-0.213	+0.079	3b
10.37269	-0.00027	+0.00179	(R^CeHsCO)	LUMO	-1.03313	-0.14256	+0.24799
-0.183	+0.011						Q

The pyrimidinium-ylides, trifluoroacetonitrile and benzoyl cyanide considered geometries and all data presented in table 1 were calculated by AM1 method¹³, using the HyperChem Program¹⁴. The correlation diagrams (figure 1) between HOMO and LUMO orbitals of ylides **1a**, respectively **2a**, and of trifluoroacetonitrile **3a**, respectively benzoyl cyanide **3b**, have been elaborated using

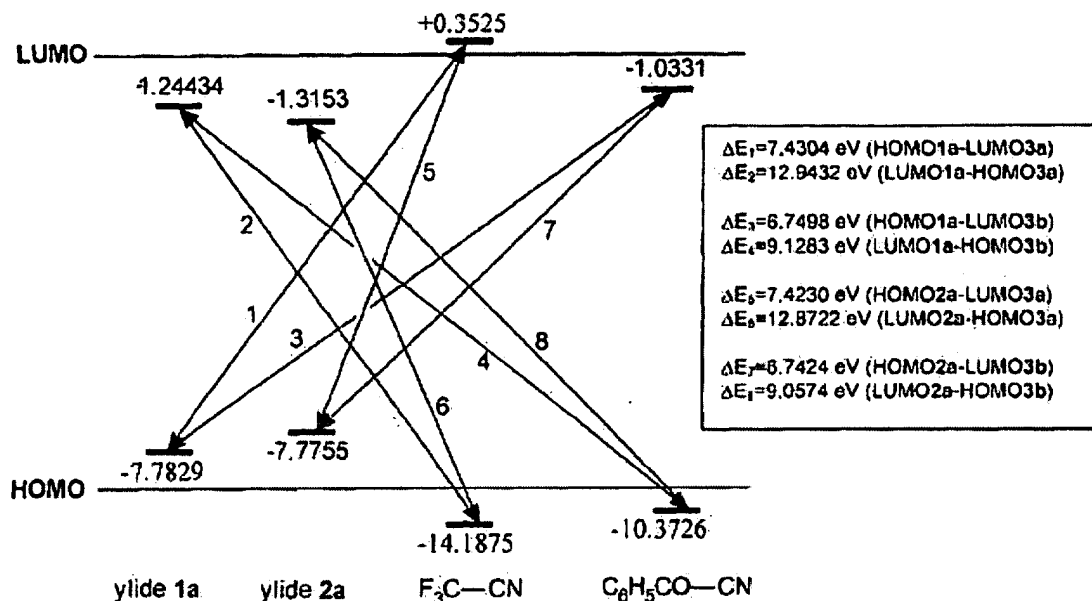


Figure 1. Correlation diagrams

According to the orbital correlation diagrams presented in figure 1, the interactions HOMO ylide - LUMO dipolarophile are characterised by the lowest interaction energies ($\Delta E_1 = 7.4304$ eV for the ylide 1a-trifluoroacetonitrile and $\Delta E_3 = 6.7498$ eV for the ylide 1a-benzoyl cyanide, respectively $\Delta E_5 = 7.4230$ eV for the ylide 2a-trifluoroacetonitrile and $\Delta E_7 = 6.7424$ eV for the ylide 2a-benzoyl cyanide). All these cycloaddition reactions are HOMO-controlled in respect to the ylide. This means that in the reaction ylide (donor) - dipolarophile (acceptor), under orbital or charge control, the most likely interaction will take place between C_3 atom of the ylide and nitrogen atom of the trifluoroacetonitrile, respectively benzoyl cyanide (figure 2).

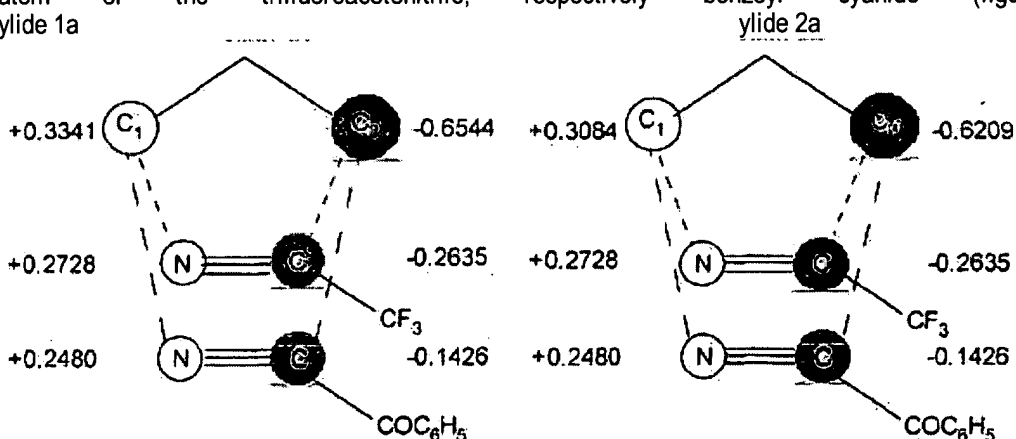


Figure 2. Graphical representation of the interaction between the frontier molecular orbitals

Taking into account that in figure 2 the atomic orbital coefficients have the same signs, the formation of A-type cycloadduct is allowed. Thus, in the case of pyrimidinium-ylides, the new bond will be realised between the ylidic carbon and the nitrogen atom from the carbon-nitrogen triple bond compounds, affording imidazo[1,2-c]pyrimidine derivatives 4-11 with A-type structures.

Conclusion

New 2,3-disubstituted imidazo [1,2-c]pyrimidine derivatives 4-11 were obtained by 1,3-dipolar cycloaddition reactions of several 4-substituted pyrimidinium-ylides, as 1,3-dipols, with activated triple bond carbon-nitrogen compounds such as trifluoroacetonitrile and benzoyl cyanide.

Analysis of all data leads to the conclusion that the [3+2] dipolar cycloaddition reactions of 4-substituted pyrimidin-2-ylides, to trifluoroacetonitrile, respectively benzoyl cyanide, are regioselective. The reactions are HOMO controlled by ylides and only one regioisomer is formed, the one in which the ylide carbanion makes the new bond with the nitrogen atom from trifluoroacetonitrile, respectively benzoyl cyanide. Thus, the theoretical and experimental data are in accordance with each other.

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